Angewandte Chemie
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Supporting Information

Pressure-Dependent Polymorphism and Band-Gap Tuning of Methylammonium Lead Iodide Perovskite

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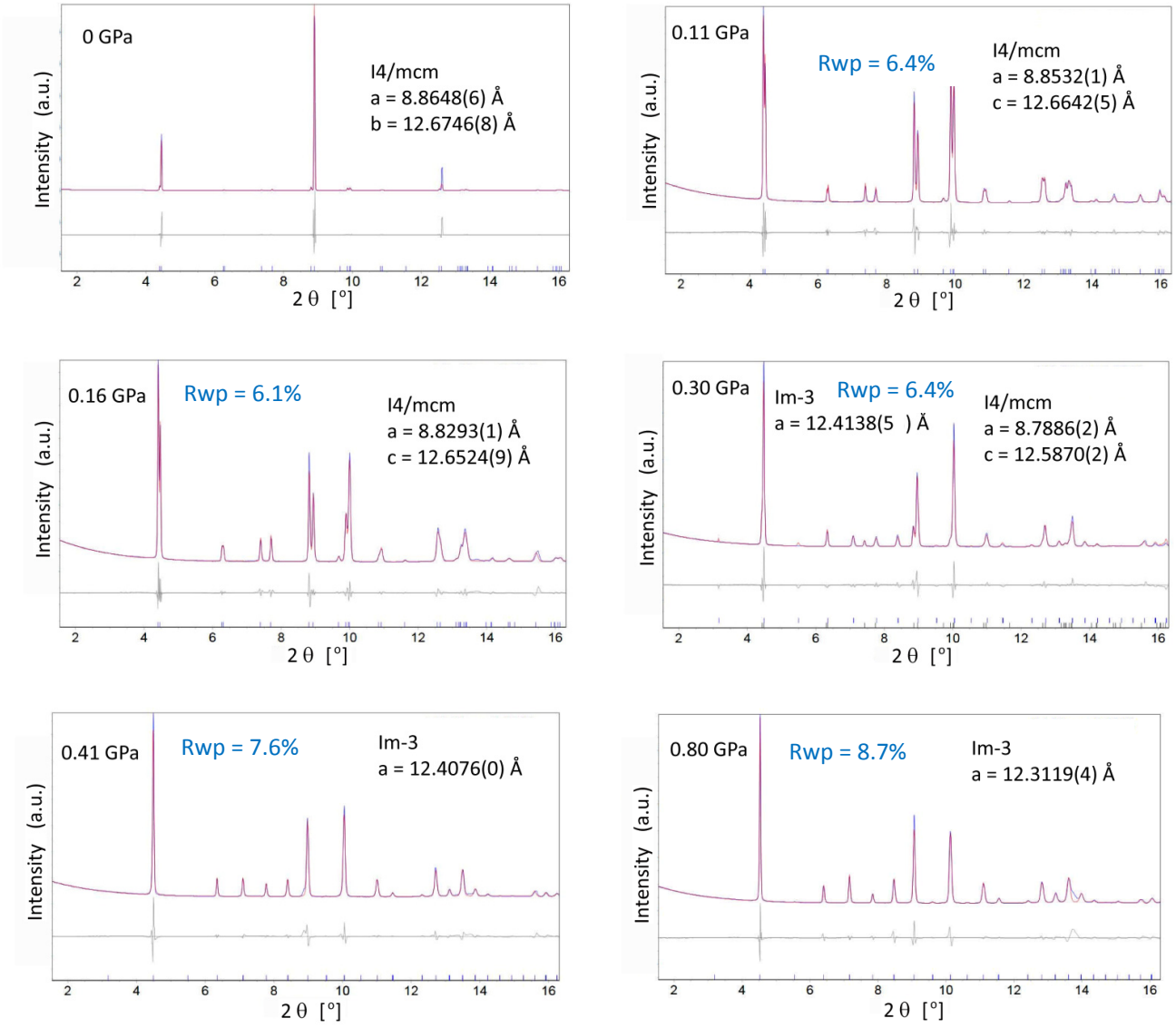
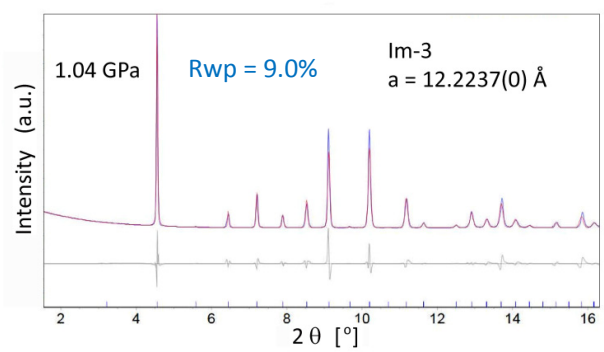
anie_201601788_sm_miscellaneous_information.pdf

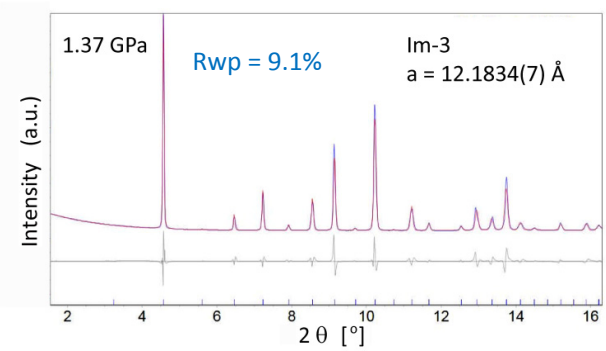
I. Results:

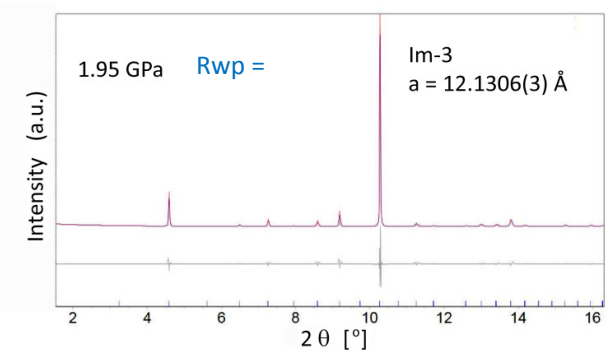
Fig. S1. Lattice parameters of $MAPbI_3$, received from Pawley fitting, during the compression and decompression runs. "Rwp" means R-weighted pattern.[S1] (Peak pressure: 6.4 GPa).

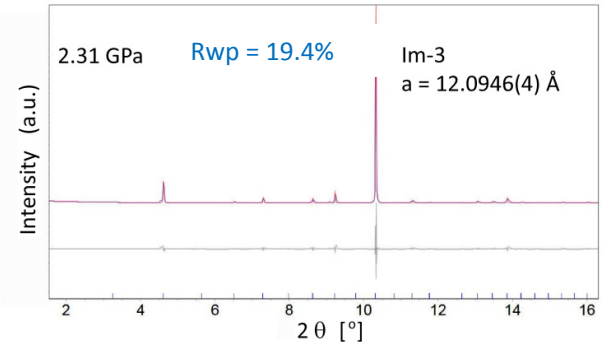
Compression:

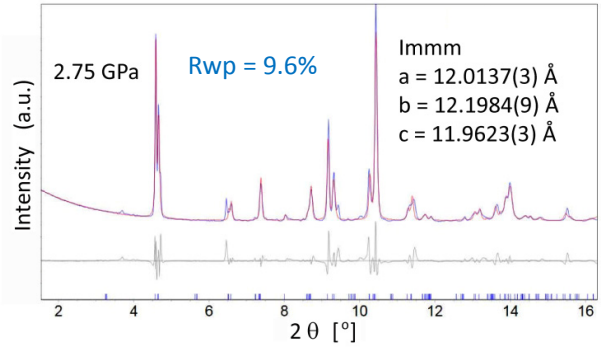


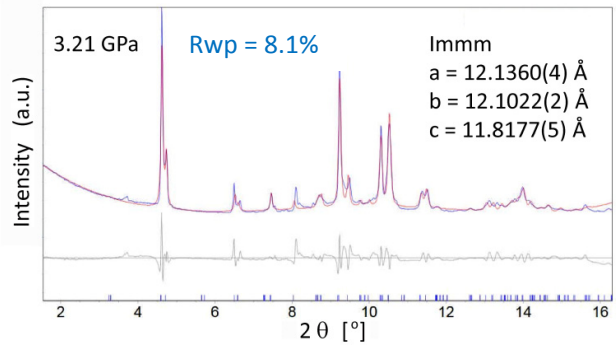




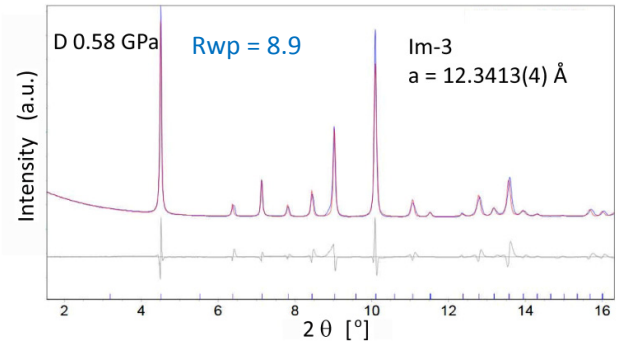








Decompression:



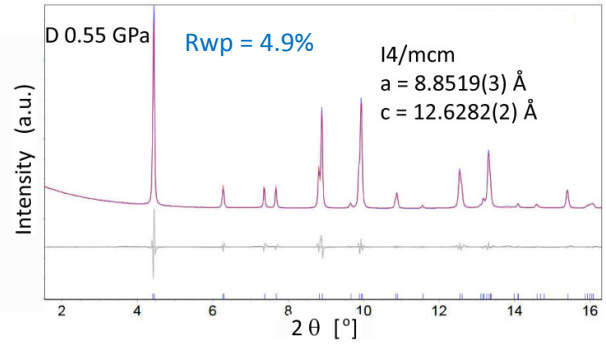
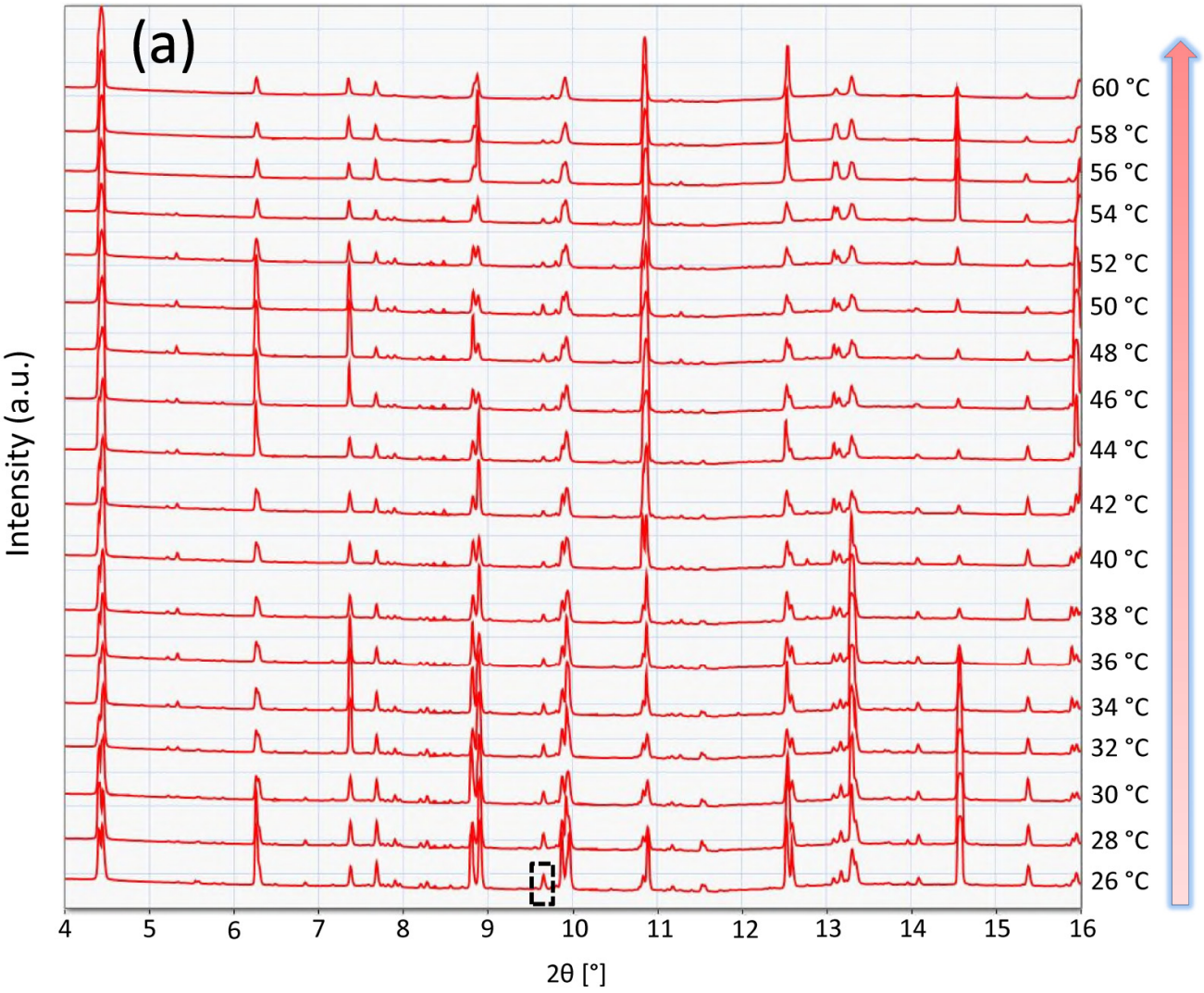


Fig. S2. Integrated synchrotron XRD pattern of $MAPbI_3$ as a function of temperature. (a) Series of patterns recorded at increasing temperatures; (b) series of patterns recorded at decreasing temperatures. The marked peaks in (a) and (b) are attributed to (123) of $MAPbI_3$ tetragonal structure.



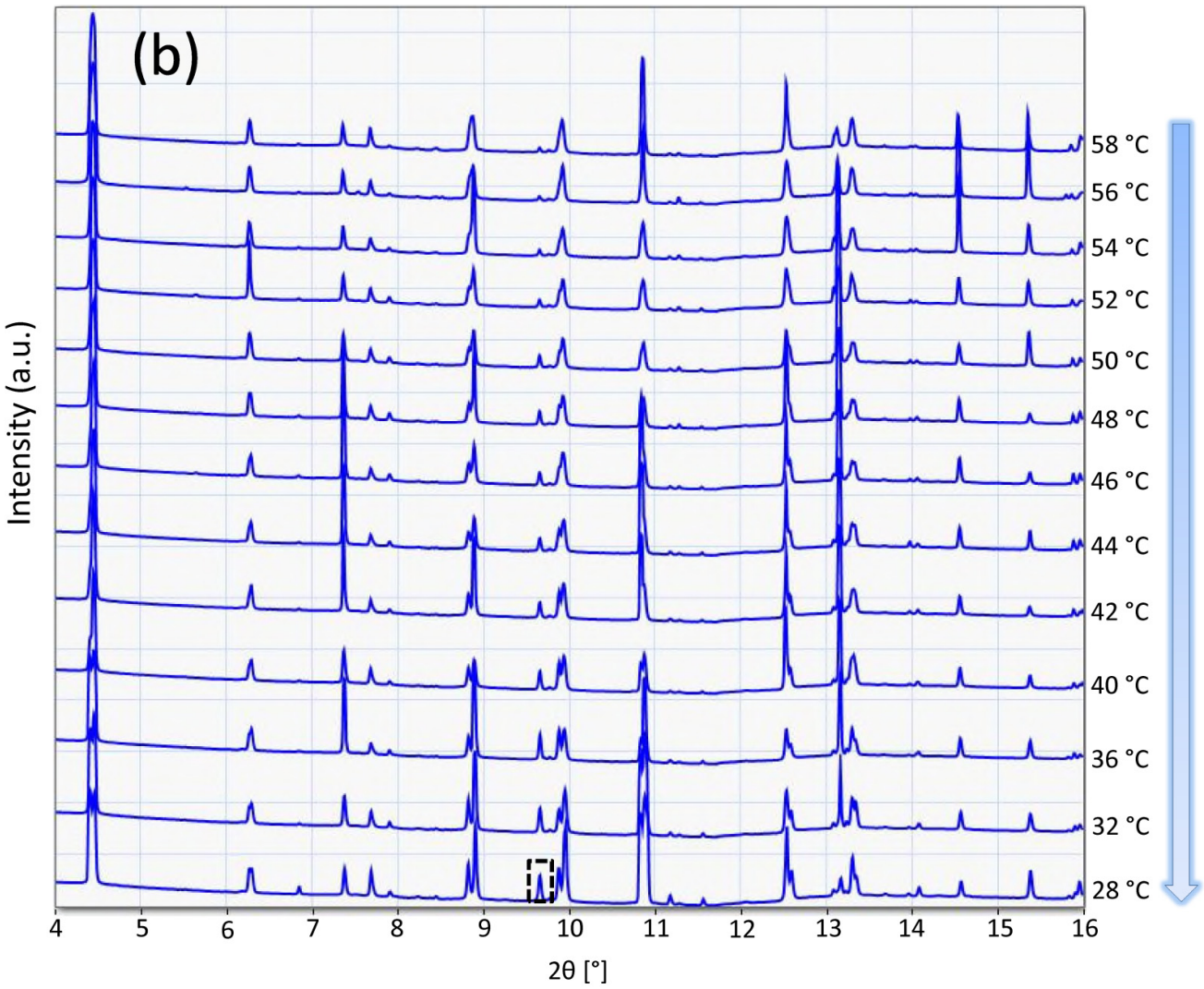
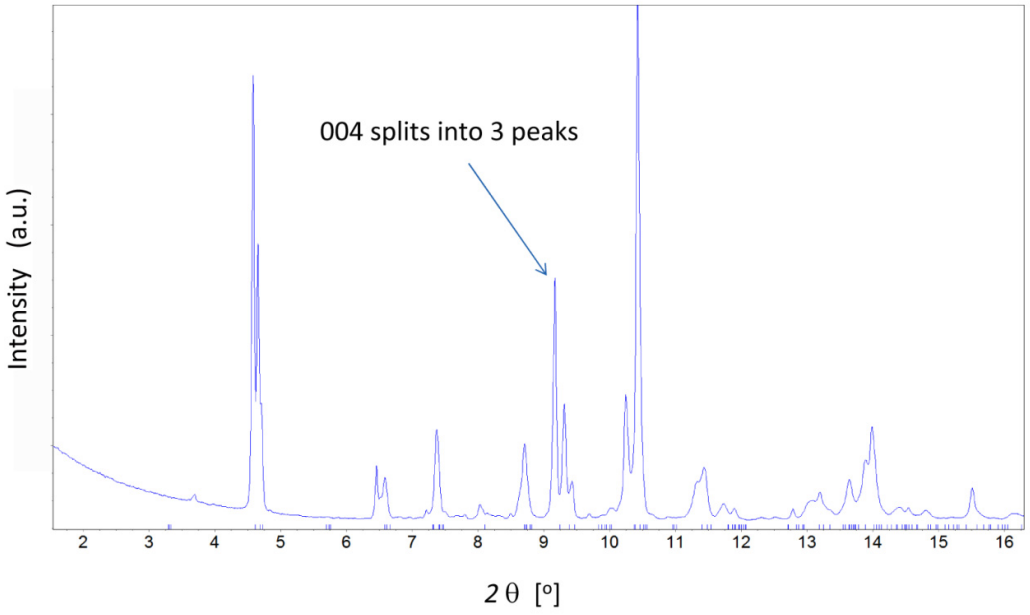

(b)
Intensity (a.u.)
58 °C
56 °C
54 °C
52 °C
50 °C
48 °C
46 °C
44 °C
42 °C
40 °C
36 °C
32 °C
28 °C
4
5
6
7
8
9
10
11
12
13
14
15
16
2θ [°]

Fig. S3. Integrated synchrotron XRD pattern of $MAPbI_3$ at pressure of 2.7_5 GPa (top) and zoon-in patterns under different pressures around $2\theta = 9^{o}$ (bottom).



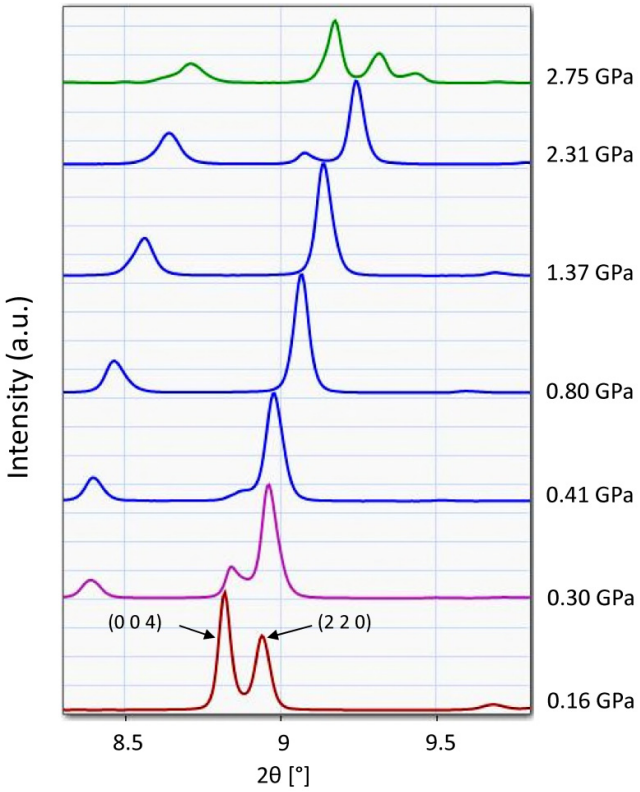


Fig. S4. Additional integrated synchrotron XRD patterns of $MAPbI_3$ (peak pressure: 3.5 GPa) during (a) compression and (b) decompression runs; and its 2D patterns during (c) compression and (d) decompression runs.

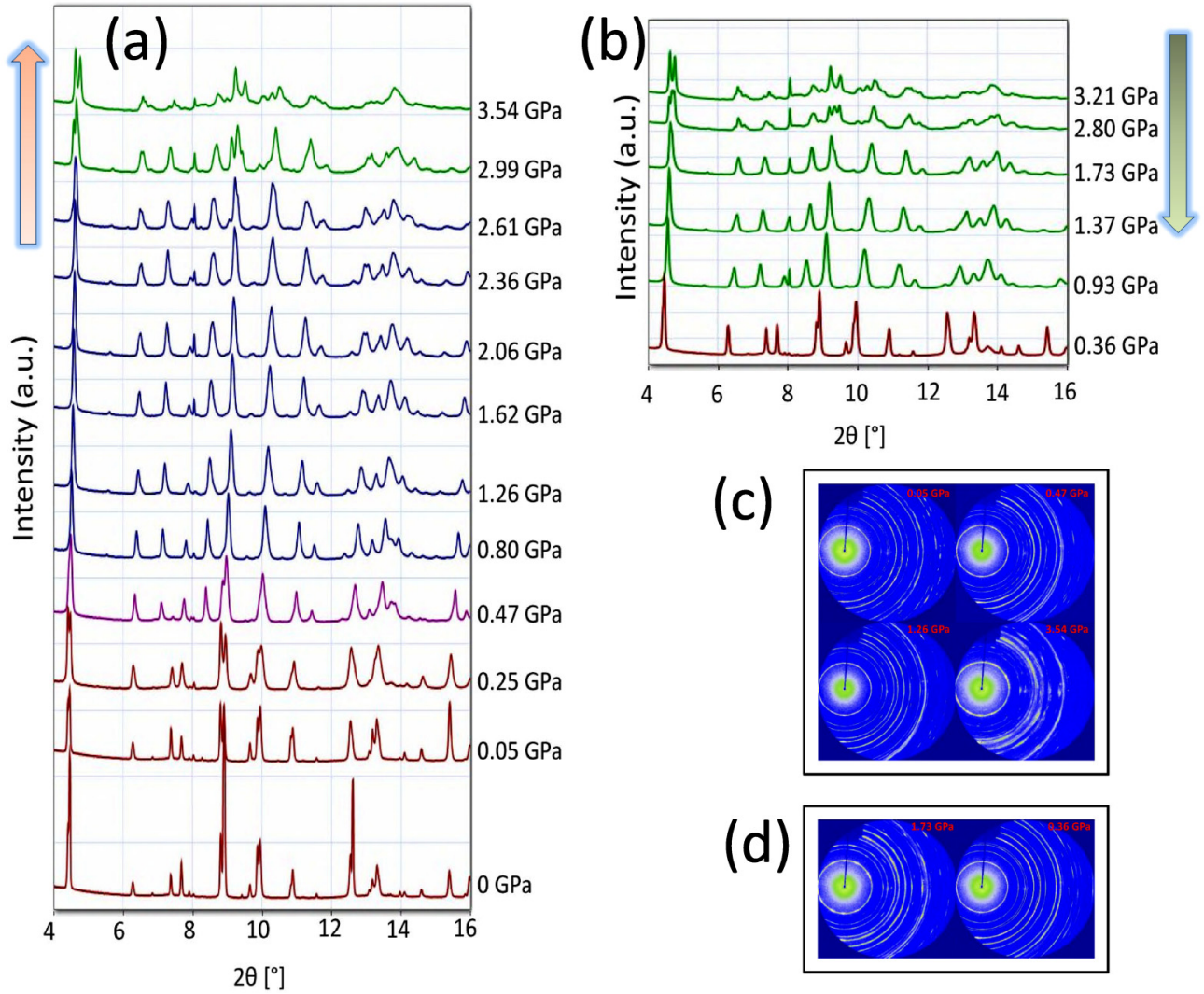
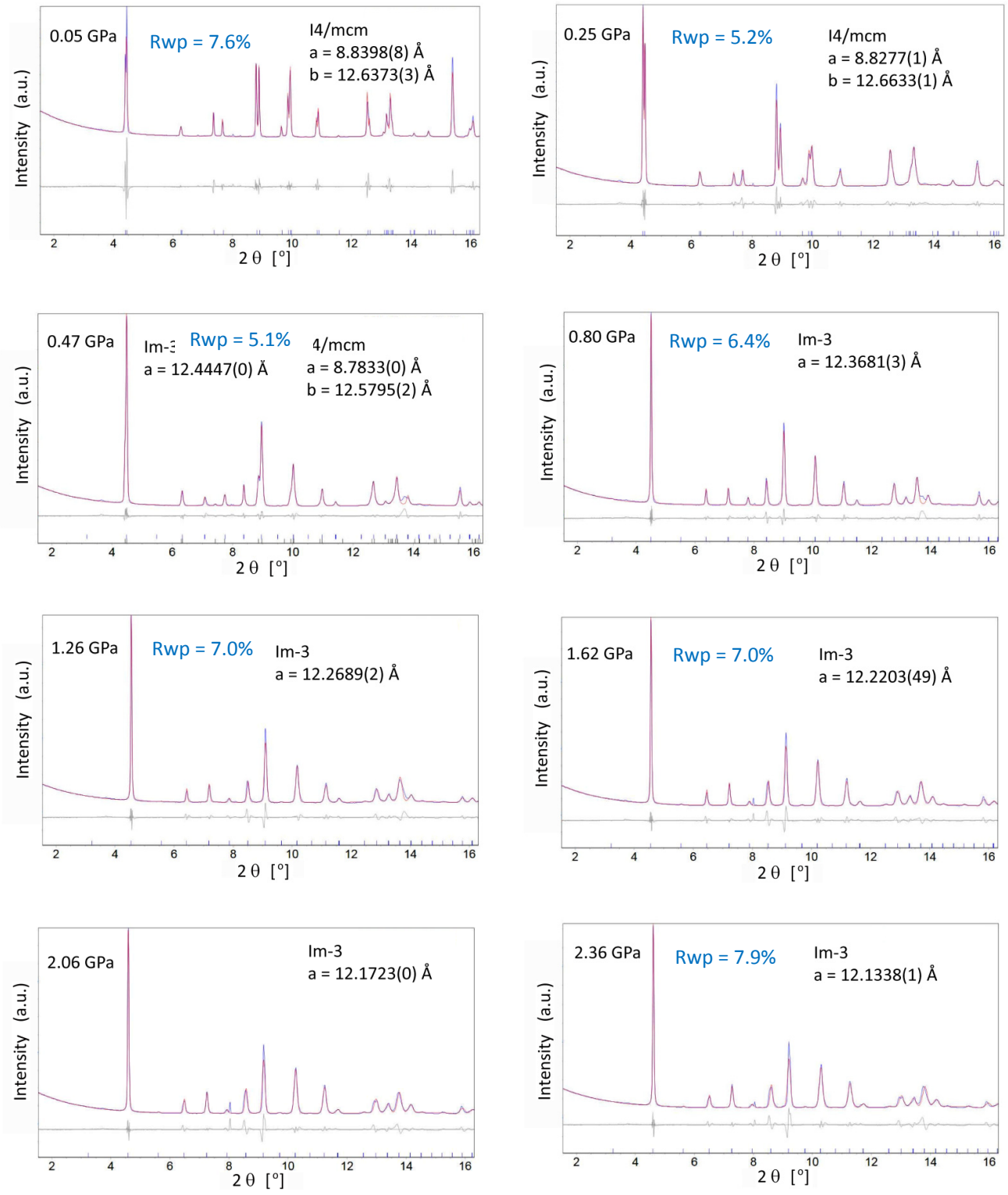
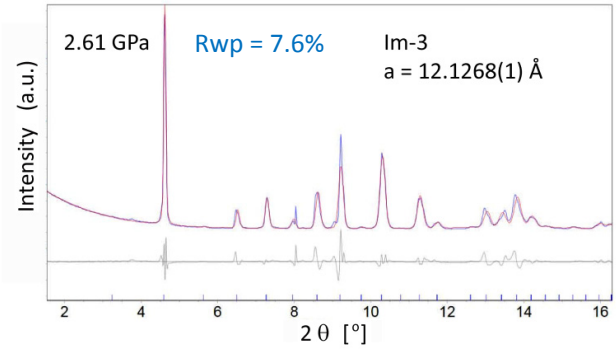
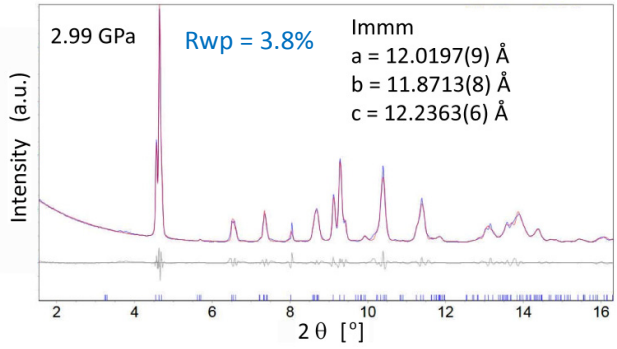


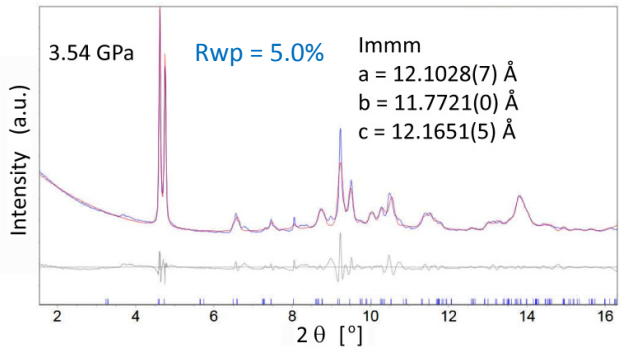
Fig. S5. Lattice parameters of $MAPbI_3$, received from Pawley fitting using data presented in Fig. S4, during the compression and decompression runs. "Rwp" means R-weighted pattern.[S2] (Peak pressure: 3.5 GPa).

Compression:

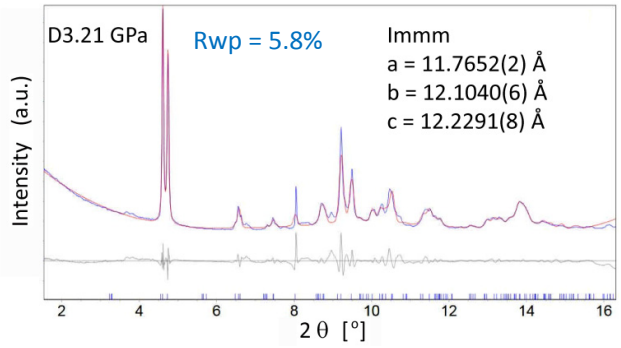


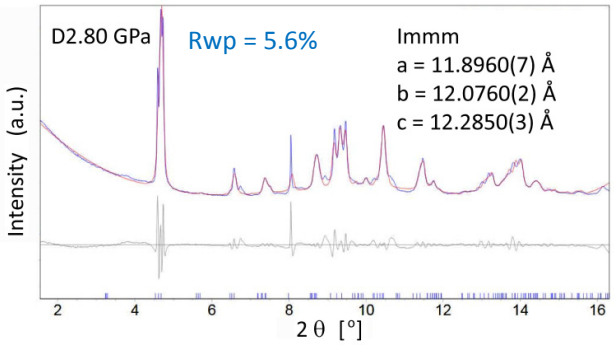

2.61 GPa
Rwp = 7.6%
Im-3
a = 12.1268(1) Å
Intensity (a.u.)
2 θ [°]

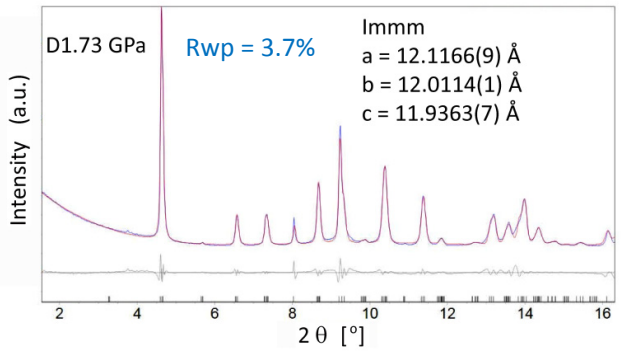

2.99 GPa
Rwp = 3.8%
Immm
a = 12.0197(9) Å
b = 11.8713(8) Å
c = 12.2363(6) Å
Intensity (a.u.)
2 θ [°]

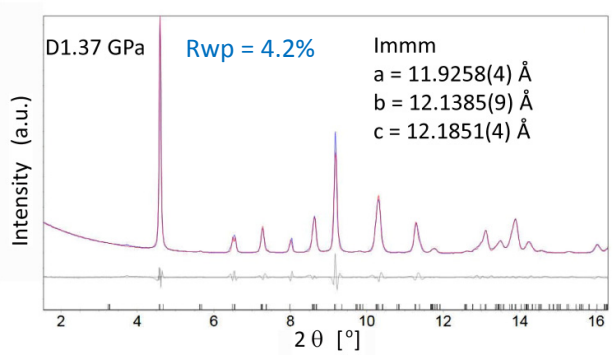

3.54 GPa
Rwp = 5.0%
Immm
a = 12.1028(7) Å
b = 11.7721(0) Å
c = 12.1651(5) Å
Intensity (a.u.)
2 θ [°]

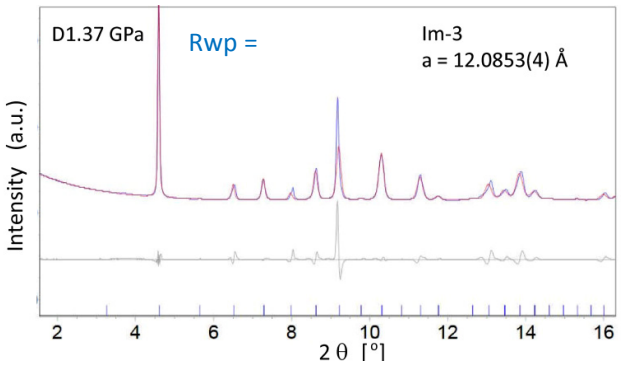
Decompression:

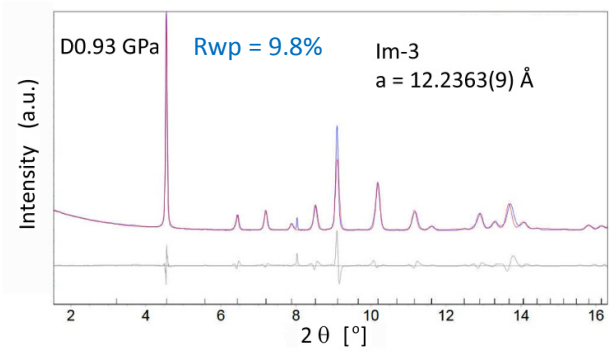












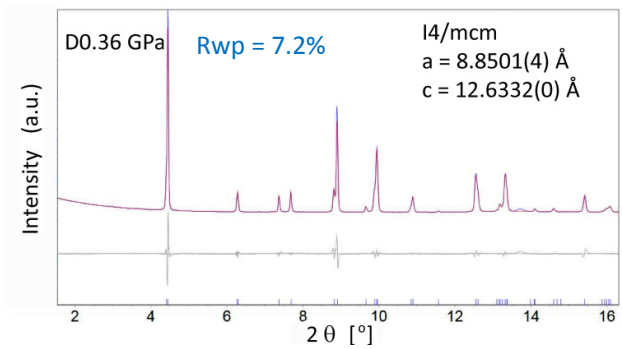


Fig. S6. Plot of unit cell volume calculated from the Pawley fittings as function of the applied pressure in two sets of compressions with different peak pressures.

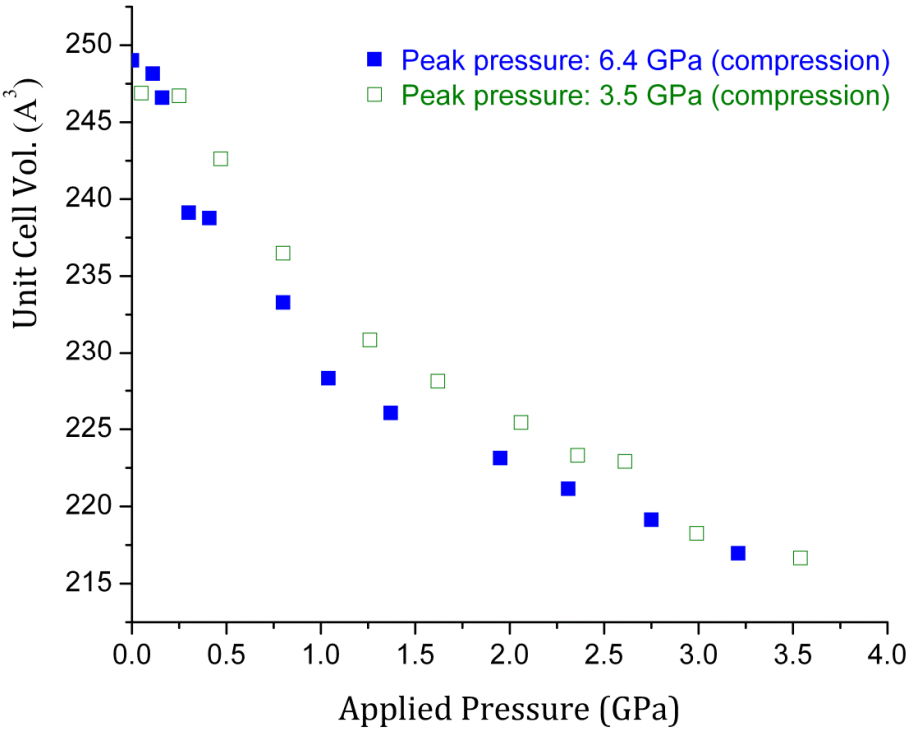


Fig. S7. Optical images of a pressed $MAPbI_3$ sample in DACs under white light. (a), compressed at 0.1_6 GPa; (b), decompressed at 3.7_1 GPa; (c), decompressed at 2.5_5 GPa; (d), decompressed at 1.9_8 GPa; and (e), decompressed to ambient pressure.

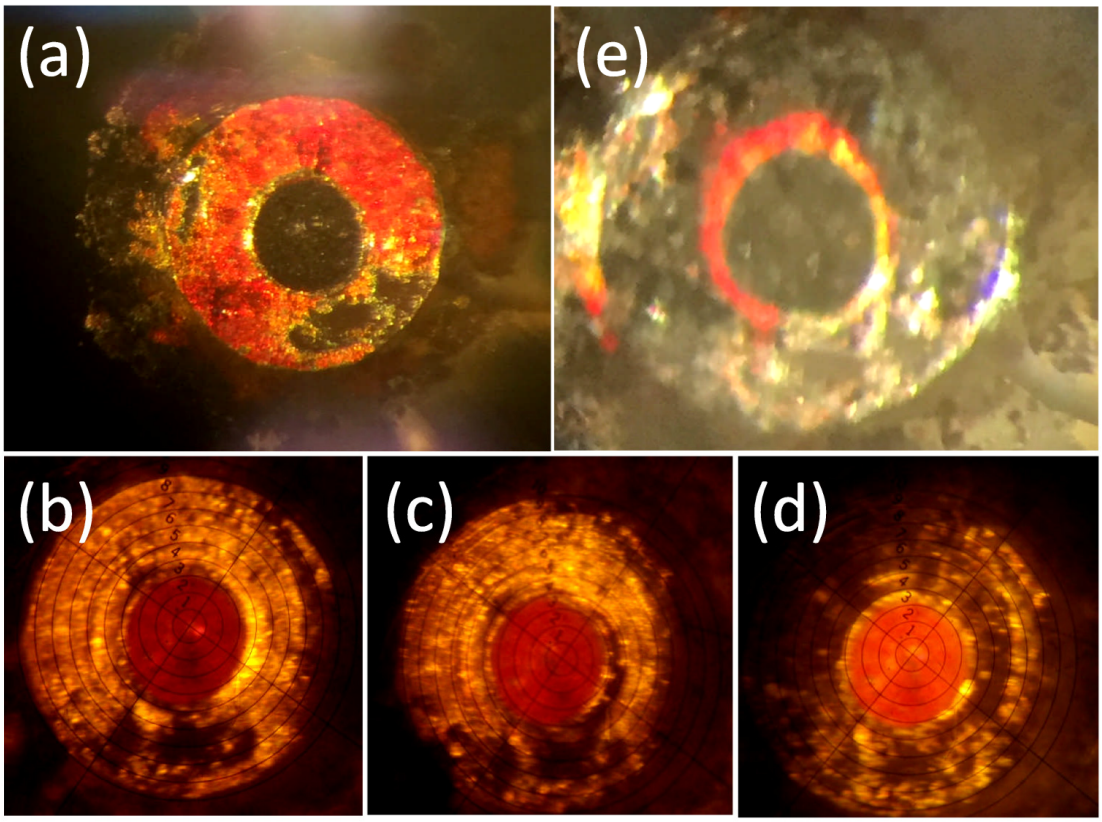


Table S1. Approximate values for the octahedral tilt angles in the cubic $Im\bar{3}$ phase using Rietveld refinements of selected data. The octahedral tilt angle was calculated using the same procedure described by Jorgensen *et al.* [ref.24]

Refined atomic positions for 0.80 GPa data

Site	Np	*x*	*y*	*z*	Atom	Occ.	Beq.
Pb1	8	0.25	0.25	0.25	Pb^{+2}	1	1
I1	24	0	0.2026(9)	0.2717(1)	I^{-1}	1	1
C/N1	2	0	0	0	Al	0.5	20
C/N2	6	0	0.5	0	Al	0.5	20

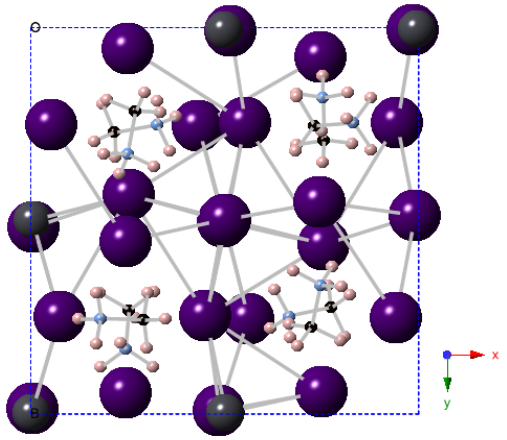
Refined atomic coordinates for I used to calculate the tilt angle (ϕ), Pb-I bond lengths and octahedral tilt angle for selected pressures.

Pressure	***y***	***z***	**Pb-I**	**ϕ**
0.8	0.2026(9)	0.2717(1)	3.145(2)	14.16
1.04	0.1961(8)	0.2705(1)	3.137(2)	15.44
1.37	0.1958(7)	0.2664(8)	3.121(2)	14.82

Table S2. Optimized cif files of tetragonal and cubic phases of $MAPbI_3$ under selected pressures.

C H I N Pb

P1_0.00GPa_tetragonal.cif



```
# CRYSTAL DATA
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_pd_phase_name                          'MAPbI3'
_cell_length_a                         12.52993
_cell_length_b                         12.52993
_cell_length_c                         12.69000
_cell_angle_alpha                      90
_cell_angle_beta                       90
_cell_angle_gamma                      90
_symmetry_space_group_name_H-M         'P 1'
_symmetry_Int_Tables_number            1

loop_
_symmetry_equiv_pos_as_xyz
   'x, y, z'

loop_
   _atom_site_label
   _atom_site_occupancy
   _atom_site_fract_x
   _atom_site_fract_y
   _atom_site_fract_z
   _atom_site_adp_type
   _atom_site_B_iso_or_equiv
   _atom_site_type_symbol
   H1          1.0     0.166330      0.293205      0.687173     Biso  1.000000 H
   H2          1.0     0.670187      0.802096      0.665659     Biso  1.000000 H
   H3          1.0     0.327476      0.188924      0.660773     Biso  1.000000 H
   H4          1.0     0.823517      0.690374      0.705330     Biso  1.000000 H
   H5          1.0     0.218981      0.336110      0.812069     Biso  1.000000 H
   H6          1.0     0.617516      0.777672      0.786272     Biso  1.000000 H
   H7          1.0     0.376969      0.230944      0.778388     Biso  1.000000 H
   H8          1.0     0.768351      0.667424      0.834178     Biso  1.000000 H
   H9          1.0     0.186213      0.198282      0.791592     Biso  1.000000 H
   H10         1.0     0.629493      0.678382      0.699345     Biso  1.000000 H
   H11         1.0     0.359017      0.317565      0.679490     Biso  1.000000 H
   H12         1.0     0.810600      0.799069      0.796890     Biso  1.000000 H
   H13         1.0     0.687274      0.302214      0.810723     Biso  1.000000 H
   H14         1.0     0.181878      0.878554      0.733732     Biso  1.000000 H
   H15         1.0     0.753859      0.124531      0.774759     Biso  1.000000 H
   H16         1.0     0.270176      0.751252      0.852404     Biso  1.000000 H
   H17         1.0     0.754952      0.348495      0.694368     Biso  1.000000 H
   H18         1.0     0.232856      0.816125      0.628817     Biso  1.000000 H
   H19         1.0     0.818622      0.168800      0.665280     Biso  1.000000 H
   H20         1.0     0.319769      0.682887      0.737488     Biso  1.000000 H
   H21         1.0     0.830235      0.300248      0.805113     Biso  1.000000 H
   H22         1.0     0.315007      0.877618      0.714341     Biso  1.000000 H
   H23         1.0     0.685539      0.171099      0.668475     Biso  1.000000 H
   H24         1.0     0.178870      0.687057      0.763486     Biso  1.000000 H
   H25         1.0     0.336059      0.219099      0.312480     Biso  1.000000 H
   H26         1.0     0.777860      0.617507      0.286519     Biso  1.000000 H
   H27         1.0     0.230966      0.377040      0.278390     Biso  1.000000 H
   H28         1.0     0.667310      0.768129      0.334311     Biso  1.000000 H
   H29         1.0     0.293381      0.166266      0.187581     Biso  1.000000 H
   H30         1.0     0.801988      0.669991      0.165759     Biso  1.000000 H
   H31         1.0     0.189192      0.327414      0.160752     Biso  1.000000 H
```

H32	1.0	0.689825	0.823076	0.205288	Biso	1.000000	H
H33	1.0	0.198269	0.186316	0.291810	Biso	1.000000	H
H34	1.0	0.678422	0.629020	0.199688	Biso	1.000000	H
H35	1.0	0.317809	0.358971	0.179732	Biso	1.000000	H
H36	1.0	0.798752	0.810690	0.296660	Biso	1.000000	H
H37	1.0	0.816770	0.234122	0.128893	Biso	1.000000	H
H38	1.0	0.348666	0.754786	0.194538	Biso	1.000000	H
H39	1.0	0.683533	0.319762	0.238767	Biso	1.000000	H
H40	1.0	0.169083	0.818517	0.164999	Biso	1.000000	H
H41	1.0	0.878983	0.181605	0.233235	Biso	1.000000	H
H42	1.0	0.302145	0.687388	0.310965	Biso	1.000000	H
H43	1.0	0.751451	0.267715	0.352912	Biso	1.000000	H
H44	1.0	0.124555	0.753958	0.274500	Biso	1.000000	H
H45	1.0	0.878117	0.315014	0.215599	Biso	1.000000	H
H46	1.0	0.300269	0.830333	0.305036	Biso	1.000000	H
H47	1.0	0.687180	0.178372	0.262086	Biso	1.000000	H
H48	1.0	0.171310	0.685438	0.168430	Biso	1.000000	H
C1	1.0	0.216554	0.271126	0.754384	Biso	1.000000	C
C2	1.0	0.756654	0.290994	0.759443	Biso	1.000000	C
C3	1.0	0.271182	0.216592	0.254680	Biso	1.000000	C
C4	1.0	0.291054	0.756656	0.259511	Biso	1.000000	C
C5	1.0	0.775137	0.724298	0.768923	Biso	1.000000	C
C6	1.0	0.254355	0.730912	0.769900	Biso	1.000000	C
C7	1.0	0.724025	0.774942	0.268919	Biso	1.000000	C
C8	1.0	0.731261	0.253595	0.270063	Biso	1.000000	C
N1	1.0	0.666376	0.747029	0.727256	Biso	1.000000	N
N2	1.0	0.245812	0.831650	0.708139	Biso	1.000000	N
N3	1.0	0.747007	0.666154	0.227435	Biso	1.000000	N
N4	1.0	0.832148	0.245880	0.208416	Biso	1.000000	N
N5	1.0	0.326915	0.250766	0.715764	Biso	1.000000	N
N6	1.0	0.753470	0.181249	0.714766	Biso	1.000000	N
N7	1.0	0.250915	0.326903	0.215874	Biso	1.000000	N
N8	1.0	0.181390	0.753441	0.214632	Biso	1.000000	N
Pb1	1.0	0.503647	-0.003304	0.493723	Biso	1.000000	Pb
Pb2	1.0	0.005405	0.498359	0.503735	Biso	1.000000	Pb
Pb3	1.0	-0.003163	0.001839	0.004716	Biso	1.000000	Pb
Pb4	1.0	0.499082	0.504473	-0.010048	Biso	1.000000	Pb
Pb5	1.0	0.498527	0.005060	0.003424	Biso	1.000000	Pb
Pb6	1.0	-0.003143	0.503500	-0.006025	Biso	1.000000	Pb
Pb7	1.0	0.001979	-0.003173	0.504717	Biso	1.000000	Pb
Pb8	1.0	0.504994	0.498873	0.489959	Biso	1.000000	Pb
I1	1.0	0.486281	-0.008682	0.751706	Biso	1.000000	I
I2	1.0	0.009363	0.515047	0.750450	Biso	1.000000	I
I3	1.0	-0.014464	0.006180	0.257600	Biso	1.000000	I
I4	1.0	0.501938	0.496439	0.241846	Biso	1.000000	I
I5	1.0	0.514798	0.009530	0.250133	Biso	1.000000	I
I6	1.0	-0.008182	0.486268	0.252066	Biso	1.000000	I
I7	1.0	0.006295	-0.014680	0.757602	Biso	1.000000	I
I8	1.0	0.497183	0.501804	0.741824	Biso	1.000000	I
I9	1.0	0.944951	0.246072	0.513741	Biso	1.000000	I
I10	1.0	0.452590	0.746575	0.513799	Biso	1.000000	I
I11	1.0	0.553213	0.245962	0.522635	Biso	1.000000	I
I12	1.0	0.074824	0.747859	0.480987	Biso	1.000000	I
I13	1.0	0.255124	0.433212	0.483011	Biso	1.000000	I
I14	1.0	0.750750	0.942234	0.534373	Biso	1.000000	I
I15	1.0	0.252294	0.054109	0.515703	Biso	1.000000	I
I16	1.0	0.755054	0.561152	0.496304	Biso	1.000000	I
I17	1.0	0.747612	0.074863	0.981093	Biso	1.000000	I
I18	1.0	0.246136	0.553153	0.022676	Biso	1.000000	I
I19	1.0	0.746750	0.452222	0.014160	Biso	1.000000	I
I20	1.0	0.245782	0.944779	0.013606	Biso	1.000000	I
I21	1.0	0.054265	0.252211	0.015697	Biso	1.000000	I
I22	1.0	0.561127	0.754506	0.996055	Biso	1.000000	I
I23	1.0	0.433115	0.254525	0.982836	Biso	1.000000	I
I24	1.0	0.942195	0.750621	0.034573	Biso	1.000000	I

P4n_0.00GPa_tetragonal.cif

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# CRYSTAL DATA

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_symmetry_Int_Tables_number            1

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   _atom_site_fract_z
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   H3          1.0     0.806429      0.681610      0.338357     Biso  1.000000 H
   H4          1.0     0.193571      0.318390      0.338357     Biso  1.000000 H
   H5          1.0     0.318390      0.806429      0.661643     Biso  1.000000 H
   H6          1.0     0.681610      0.193571      0.661643     Biso  1.000000 H
   H7          1.0     0.693571      0.818390      0.661643     Biso  1.000000 H
   H8          1.0     0.306429      0.181610      0.661643     Biso  1.000000 H
   H9          1.0     0.122335      0.728502      0.222601     Biso  1.000000 H
   H10         1.0     0.877665      0.271498      0.222601     Biso  1.000000 H
   H11         1.0     0.771498      0.622335      0.222601     Biso  1.000000 H
   H12         1.0     0.228502      0.377665      0.222601     Biso  1.000000 H
   H13         1.0     0.377665      0.771498      0.777399     Biso  1.000000 H
   H14         1.0     0.622335      0.228502      0.777399     Biso  1.000000 H
   H15         1.0     0.728502      0.877665      0.777399     Biso  1.000000 H
   H16         1.0     0.271498      0.122335      0.777399     Biso  1.000000 H
   H17         1.0     0.160825      0.822237      0.308807     Biso  1.000000 H
   H18         1.0     0.839175      0.177763      0.308807     Biso  1.000000 H
   H19         1.0     0.677763      0.660825      0.308807     Biso  1.000000 H
   H20         1.0     0.322237      0.339175      0.308807     Biso  1.000000 H
   H21         1.0     0.339175      0.677763      0.691193     Biso  1.000000 H
   H22         1.0     0.660825      0.322237      0.691193     Biso  1.000000 H
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   H24         1.0     0.177763      0.160825      0.691193     Biso  1.000000 H
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   H26         1.0     0.717008      0.191565      0.157760     Biso  1.000000 H
   H27         1.0     0.691565      0.782992      0.157760     Biso  1.000000 H
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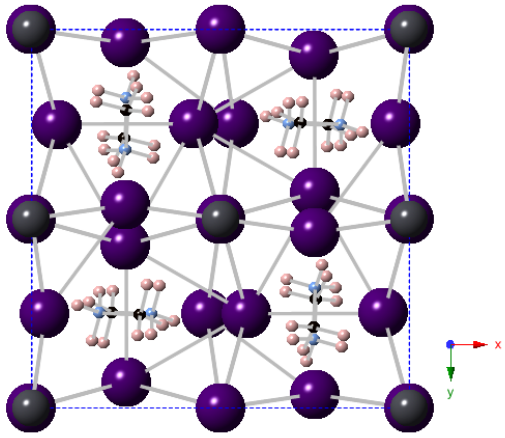

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H40	1.0	0.326905	0.307431	0.803980	Biso	1.000000 H
H41	1.0	0.347269	0.780460	0.281380	Biso	1.000000 H
H42	1.0	0.652731	0.219540	0.281380	Biso	1.000000 H
H43	1.0	0.719540	0.847269	0.281380	Biso	1.000000 H
H44	1.0	0.280460	0.152731	0.281380	Biso	1.000000 H
H45	1.0	0.152731	0.719540	0.718620	Biso	1.000000 H
H46	1.0	0.847269	0.280460	0.718620	Biso	1.000000 H
H47	1.0	0.780460	0.652731	0.718620	Biso	1.000000 H
H48	1.0	0.219540	0.347269	0.718620	Biso	1.000000 H
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C2	1.0	0.712420	0.246834	0.224444	Biso	1.000000 C
C3	1.0	0.746834	0.787580	0.224444	Biso	1.000000 C
C4	1.0	0.253166	0.212420	0.224444	Biso	1.000000 C
C5	1.0	0.212420	0.746834	0.775556	Biso	1.000000 C
C6	1.0	0.787580	0.253166	0.775556	Biso	1.000000 C
C7	1.0	0.753166	0.712420	0.775556	Biso	1.000000 C
C8	1.0	0.246834	0.287580	0.775556	Biso	1.000000 C
N1	1.0	0.181354	0.748909	0.277070	Biso	1.000000 N
N2	1.0	0.818646	0.251091	0.277070	Biso	1.000000 N
N3	1.0	0.751091	0.681354	0.277070	Biso	1.000000 N
N4	1.0	0.248909	0.318646	0.277070	Biso	1.000000 N
N5	1.0	0.318646	0.751091	0.722930	Biso	1.000000 N
N6	1.0	0.681354	0.248909	0.722930	Biso	1.000000 N
N7	1.0	0.748909	0.818646	0.722930	Biso	1.000000 N
N8	1.0	0.251091	0.181354	0.722930	Biso	1.000000 N
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Pb2	1.0	0.500000	0.500000	0.500000	Biso	1.000000 Pb
Pb3	1.0	0.500000	0.000000	-0.009160	Biso	1.000000 Pb
Pb4	1.0	0.000000	0.500000	0.009160	Biso	1.000000 Pb
Pb5	1.0	0.500000	0.000000	0.482956	Biso	1.000000 Pb
Pb6	1.0	0.000000	0.500000	0.517044	Biso	1.000000 Pb
Pb7	1.0	0.000000	0.000000	-0.000000	Biso	1.000000 Pb
Pb8	1.0	0.500000	0.500000	-0.000000	Biso	1.000000 Pb
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I2	1.0	0.568670	0.750510	0.502664	Biso	1.000000 I
I3	1.0	0.250510	0.931330	0.502664	Biso	1.000000 I
I4	1.0	0.749490	0.068670	0.502664	Biso	1.000000 I
I5	1.0	0.068670	0.250510	0.497336	Biso	1.000000 I
I6	1.0	0.931330	0.749490	0.497336	Biso	1.000000 I
I7	1.0	0.249490	0.568670	0.497336	Biso	1.000000 I
I8	1.0	0.750510	0.431330	0.497336	Biso	1.000000 I
I9	1.0	0.249898	0.036436	0.965710	Biso	1.000000 I
I10	1.0	0.750102	0.963564	0.965710	Biso	1.000000 I
I11	1.0	0.463564	0.749898	0.965710	Biso	1.000000 I
I12	1.0	0.536436	0.250102	0.965710	Biso	1.000000 I
I13	1.0	0.250102	0.463564	0.034290	Biso	1.000000 I
I14	1.0	0.749898	0.536436	0.034290	Biso	1.000000 I
I15	1.0	0.036436	0.750102	0.034290	Biso	1.000000 I
I16	1.0	0.963564	0.249898	0.034290	Biso	1.000000 I
I17	1.0	0.500000	0.000000	0.237231	Biso	1.000000 I
I18	1.0	0.000000	0.500000	0.762769	Biso	1.000000 I
I19	1.0	0.000000	0.000000	0.747113	Biso	1.000000 I
I20	1.0	0.500000	0.500000	0.747113	Biso	1.000000 I
I21	1.0	0.500000	0.500000	0.252887	Biso	1.000000 I
I22	1.0	0.000000	0.000000	0.252887	Biso	1.000000 I
I23	1.0	0.000000	0.500000	0.266156	Biso	1.000000 I
I24	1.0	0.500000	0.000000	0.733844	Biso	1.000000 I

P1_0.30GPa_tetragonal.cif

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# CRYSTAL DATA

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   H4          1.0     0.824607     0.692484     0.707812     Biso  1.000000 H
   H5          1.0     0.215106     0.335622     0.810735     Biso  1.000000 H
   H6          1.0     0.616239     0.776808     0.790727     Biso  1.000000 H
   H7          1.0     0.377059     0.233133     0.778076     Biso  1.000000 H
   H8          1.0     0.769836     0.666929     0.837487     Biso  1.000000 H
   H9          1.0     0.186225     0.195564     0.792750     Biso  1.000000 H
   H10         1.0     0.628669     0.676559     0.703447     Biso  1.000000 H
   H11         1.0     0.356210     0.318816     0.677338     Biso  1.000000 H
   H12         1.0     0.809698     0.800587     0.801160     Biso  1.000000 H
   H13         1.0     0.687321     0.304393     0.811170     Biso  1.000000 H
   H14         1.0     0.181901     0.879059     0.734064     Biso  1.000000 H
   H15         1.0     0.753380     0.124639     0.778760     Biso  1.000000 H
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   H19         1.0     0.819174     0.166516     0.667651     Biso  1.000000 H
   H20         1.0     0.325425     0.685500     0.744192     Biso  1.000000 H
   H21         1.0     0.831295     0.301958     0.805722     Biso  1.000000 H
   H22         1.0     0.316714     0.880765     0.719673     Biso  1.000000 H
   H23         1.0     0.685083     0.169581     0.670724     Biso  1.000000 H
   H24         1.0     0.182384     0.685552     0.763610     Biso  1.000000 H
   H25         1.0     0.335478     0.215227     0.311170     Biso  1.000000 H
   H26         1.0     0.777038     0.616425     0.290870     Biso  1.000000 H
   H27         1.0     0.233059     0.377133     0.278165     Biso  1.000000 H
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   H31         1.0     0.188321     0.328101     0.160466     Biso  1.000000 H
   H32         1.0     0.691811     0.824297     0.207643     Biso  1.000000 H
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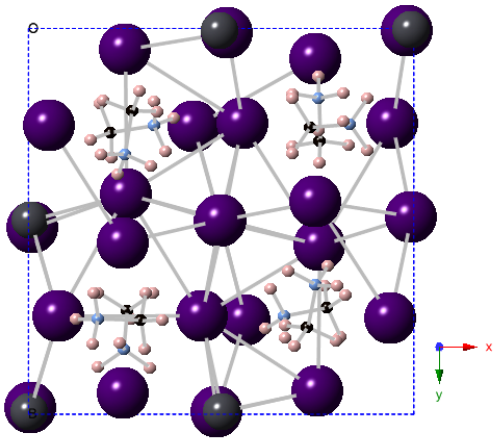

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H37	1.0	0.817626	0.239614	0.130739	Biso	1.000000	H
H38	1.0	0.348787	0.755251	0.193285	Biso	1.000000	H
H39	1.0	0.685558	0.324794	0.244717	Biso	1.000000	H
H40	1.0	0.166898	0.819062	0.167273	Biso	1.000000	H
H41	1.0	0.879550	0.181913	0.233928	Biso	1.000000	H
H42	1.0	0.304364	0.687273	0.311250	Biso	1.000000	H
H43	1.0	0.752563	0.265814	0.357252	Biso	1.000000	H
H44	1.0	0.124727	0.753494	0.278430	Biso	1.000000	H
H45	1.0	0.880842	0.316925	0.220739	Biso	1.000000	H
H46	1.0	0.302086	0.831251	0.305562	Biso	1.000000	H
H47	1.0	0.685798	0.181516	0.262189	Biso	1.000000	H
H48	1.0	0.169792	0.684962	0.170583	Biso	1.000000	H
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C3	1.0	0.269036	0.214521	0.254140	Biso	1.000000	C
C4	1.0	0.291995	0.757077	0.259767	Biso	1.000000	C
C5	1.0	0.775364	0.724936	0.772303	Biso	1.000000	C
C6	1.0	0.256655	0.731989	0.773519	Biso	1.000000	C
C7	1.0	0.724591	0.775327	0.272177	Biso	1.000000	C
C8	1.0	0.732018	0.255686	0.273374	Biso	1.000000	C
N1	1.0	0.665320	0.746268	0.730994	Biso	1.000000	N
N2	1.0	0.248209	0.833054	0.710876	Biso	1.000000	N
N3	1.0	0.746298	0.665283	0.231054	Biso	1.000000	N
N4	1.0	0.833422	0.248272	0.211143	Biso	1.000000	N
N5	1.0	0.325955	0.251132	0.714994	Biso	1.000000	N
N6	1.0	0.753565	0.180449	0.717107	Biso	1.000000	N
N7	1.0	0.251192	0.325978	0.215154	Biso	1.000000	N
N8	1.0	0.180662	0.753502	0.216882	Biso	1.000000	N
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Pb2	1.0	0.006540	0.497332	0.505904	Biso	1.000000	Pb
Pb3	1.0	-0.005090	0.002117	0.006568	Biso	1.000000	Pb
Pb4	1.0	0.498088	0.505395	-0.008205	Biso	1.000000	Pb
Pb5	1.0	0.497233	0.005883	0.005704	Biso	1.000000	Pb
Pb6	1.0	-0.004493	0.503379	-0.004221	Biso	1.000000	Pb
Pb7	1.0	0.002249	-0.004962	0.506590	Biso	1.000000	Pb
Pb8	1.0	0.506020	0.497771	0.491853	Biso	1.000000	Pb
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I2	1.0	0.010718	0.516262	0.751559	Biso	1.000000	I
I3	1.0	-0.016417	0.004729	0.258110	Biso	1.000000	I
I4	1.0	0.500933	0.496599	0.243430	Biso	1.000000	I
I5	1.0	0.515588	0.010807	0.251383	Biso	1.000000	I
I6	1.0	-0.005246	0.488227	0.253539	Biso	1.000000	I
I7	1.0	0.004845	-0.016203	0.758162	Biso	1.000000	I
I8	1.0	0.497104	0.500535	0.743447	Biso	1.000000	I
I9	1.0	0.945045	0.245310	0.514945	Biso	1.000000	I
I10	1.0	0.449963	0.745621	0.516129	Biso	1.000000	I
I11	1.0	0.555253	0.245512	0.523078	Biso	1.000000	I
I12	1.0	0.078214	0.746622	0.484095	Biso	1.000000	I
I13	1.0	0.255363	0.429361	0.484411	Biso	1.000000	I
I14	1.0	0.750818	0.939420	0.535922	Biso	1.000000	I
I15	1.0	0.252222	0.054375	0.514869	Biso	1.000000	I
I16	1.0	0.755518	0.562472	0.499965	Biso	1.000000	I
I17	1.0	0.746601	0.077681	0.984221	Biso	1.000000	I
I18	1.0	0.245936	0.555334	0.022960	Biso	1.000000	I
I19	1.0	0.746052	0.449532	0.016228	Biso	1.000000	I
I20	1.0	0.245206	0.945024	0.014993	Biso	1.000000	I
I21	1.0	0.054554	0.252155	0.014746	Biso	1.000000	I
I22	1.0	0.562391	0.755009	0.999847	Biso	1.000000	I
I23	1.0	0.429514	0.254929	0.984328	Biso	1.000000	I
I24	1.0	0.939465	0.750700	0.035991	Biso	1.000000	I

P4n_0.30GPa_tetragonal.cif

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#======================================================================

# CRYSTAL DATA

#----------------------------------------------------------------------

data_VESTA_phase_1


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_cell_length_b                         12.43094
_cell_length_c                         12.60000
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_cell_angle_beta                       90
_cell_angle_gamma                      90
_symmetry_space_group_name_H-M         'P 1'
_symmetry_Int_Tables_number            1

loop_
_symmetry_equiv_pos_as_xyz
   'x, y, z'

loop_
   _atom_site_label
   _atom_site_occupancy
   _atom_site_fract_x
   _atom_site_fract_y
   _atom_site_fract_z
   _atom_site_adp_type
   _atom_site_B_iso_or_equiv
   _atom_site_type_symbol
   H1         1.0     0.180888     0.691804     0.335890     Biso  1.000000 H
   H2         1.0     0.819112     0.308196     0.335890     Biso  1.000000 H
   H3         1.0     0.808196     0.680888     0.335890     Biso  1.000000 H
   H4         1.0     0.191804     0.319112     0.335890     Biso  1.000000 H
   H5         1.0     0.319112     0.808196     0.664110     Biso  1.000000 H
   H6         1.0     0.680888     0.191804     0.664110     Biso  1.000000 H
   H7         1.0     0.691804     0.819112     0.664110     Biso  1.000000 H
   H8         1.0     0.308196     0.180888     0.664110     Biso  1.000000 H
   H9         1.0     0.116854     0.728975     0.222234     Biso  1.000000 H
   H10        1.0     0.883146     0.271025     0.222234     Biso  1.000000 H
   H11        1.0     0.771025     0.616854     0.222234     Biso  1.000000 H
   H12        1.0     0.228975     0.383146     0.222234     Biso  1.000000 H
   H13        1.0     0.383146     0.771025     0.777766     Biso  1.000000 H
   H14        1.0     0.616854     0.228975     0.777766     Biso  1.000000 H
   H15        1.0     0.728975     0.883146     0.777766     Biso  1.000000 H
   H16        1.0     0.271025     0.116854     0.777766     Biso  1.000000 H
   H17        1.0     0.153531     0.821478     0.312066     Biso  1.000000 H
   H18        1.0     0.846469     0.178522     0.312066     Biso  1.000000 H
   H19        1.0     0.678522     0.653531     0.312066     Biso  1.000000 H
   H20        1.0     0.321478     0.346469     0.312066     Biso  1.000000 H
   H21        1.0     0.346469     0.678522     0.687934     Biso  1.000000 H
   H22        1.0     0.653531     0.321478     0.687934     Biso  1.000000 H
   H23        1.0     0.821478     0.846469     0.687934     Biso  1.000000 H
   H24        1.0     0.178522     0.153531     0.687934     Biso  1.000000 H
   H25        1.0     0.273631     0.822640     0.159167     Biso  1.000000 H
   H26        1.0     0.726369     0.177360     0.159167     Biso  1.000000 H
   H27        1.0     0.677360     0.773631     0.159167     Biso  1.000000 H
   H28        1.0     0.322640     0.226369     0.159167     Biso  1.000000 H
   H29        1.0     0.226369     0.677360     0.840833     Biso  1.000000 H
   H30        1.0     0.773631     0.322640     0.840833     Biso  1.000000 H
   H31        1.0     0.822640     0.726369     0.840833     Biso  1.000000 H
   H32        1.0     0.177360     0.273631     0.840833     Biso  1.000000 H
   H33        1.0     0.303137     0.684205     0.185508     Biso  1.000000 H
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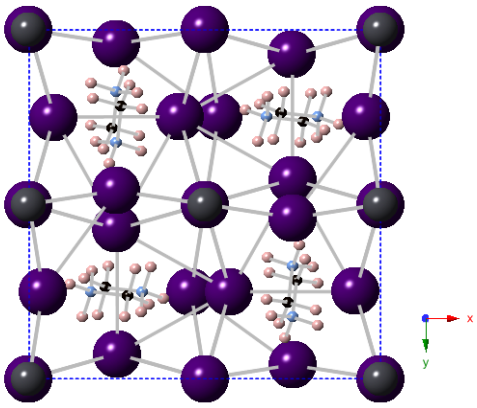

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H35	1.0	0.815795	0.803137	0.185508	Biso	1.000000	H
H36	1.0	0.184205	0.196863	0.185508	Biso	1.000000	H
H37	1.0	0.196863	0.815795	0.814492	Biso	1.000000	H
H38	1.0	0.803137	0.184205	0.814492	Biso	1.000000	H
H39	1.0	0.684205	0.696863	0.814492	Biso	1.000000	H
H40	1.0	0.315795	0.303137	0.814492	Biso	1.000000	H
H41	1.0	0.342949	0.786183	0.279005	Biso	1.000000	H
H42	1.0	0.657051	0.213817	0.279005	Biso	1.000000	H
H43	1.0	0.713817	0.842949	0.279005	Biso	1.000000	H
H44	1.0	0.286183	0.157051	0.279005	Biso	1.000000	H
H45	1.0	0.157051	0.713817	0.720995	Biso	1.000000	H
H46	1.0	0.842949	0.286183	0.720995	Biso	1.000000	H
H47	1.0	0.786183	0.657051	0.720995	Biso	1.000000	H
H48	1.0	0.213817	0.342949	0.720995	Biso	1.000000	H
C1	1.0	0.281841	0.761591	0.221292	Biso	1.000000	C
C2	1.0	0.718159	0.238409	0.221292	Biso	1.000000	C
C3	1.0	0.738409	0.781841	0.221292	Biso	1.000000	C
C4	1.0	0.261591	0.218160	0.221292	Biso	1.000000	C
C5	1.0	0.218160	0.738409	0.778708	Biso	1.000000	C
C6	1.0	0.781841	0.261591	0.778708	Biso	1.000000	C
C7	1.0	0.761591	0.718159	0.778708	Biso	1.000000	C
C8	1.0	0.238409	0.281841	0.778708	Biso	1.000000	C
N1	1.0	0.176614	0.749974	0.276542	Biso	1.000000	N
N2	1.0	0.823386	0.250026	0.276542	Biso	1.000000	N
N3	1.0	0.750026	0.676614	0.276542	Biso	1.000000	N
N4	1.0	0.249974	0.323386	0.276542	Biso	1.000000	N
N5	1.0	0.323386	0.750026	0.723458	Biso	1.000000	N
N6	1.0	0.676614	0.249974	0.723458	Biso	1.000000	N
N7	1.0	0.749974	0.823386	0.723458	Biso	1.000000	N
N8	1.0	0.250026	0.176614	0.723458	Biso	1.000000	N
Pb1	1.0	-0.000000	0.000000	0.500000	Biso	1.000000	Pb
Pb2	1.0	0.500000	0.500000	0.500000	Biso	1.000000	Pb
Pb3	1.0	0.500000	0.000000	-0.005810	Biso	1.000000	Pb
Pb4	1.0	-0.000000	0.500000	0.005810	Biso	1.000000	Pb
Pb5	1.0	0.500000	0.000000	0.485367	Biso	1.000000	Pb
Pb6	1.0	-0.000000	0.500000	0.514633	Biso	1.000000	Pb
Pb7	1.0	-0.000000	0.000000	-0.000000	Biso	1.000000	Pb
Pb8	1.0	0.500000	0.500000	-0.000000	Biso	1.000000	Pb
I1	1.0	0.428700	0.249695	0.502562	Biso	1.000000	I
I2	1.0	0.571300	0.750305	0.502562	Biso	1.000000	I
I3	1.0	0.250305	0.928700	0.502562	Biso	1.000000	I
I4	1.0	0.749695	0.071300	0.502562	Biso	1.000000	I
I5	1.0	0.071300	0.250305	0.497438	Biso	1.000000	I
I6	1.0	0.928700	0.749695	0.497438	Biso	1.000000	I
I7	1.0	0.249695	0.571300	0.497438	Biso	1.000000	I
I8	1.0	0.750305	0.428700	0.497438	Biso	1.000000	I
I9	1.0	0.249978	0.039058	0.972936	Biso	1.000000	I
I10	1.0	0.750022	0.960942	0.972936	Biso	1.000000	I
I11	1.0	0.460942	0.749978	0.972936	Biso	1.000000	I
I12	1.0	0.539058	0.250022	0.972936	Biso	1.000000	I
I13	1.0	0.250022	0.460942	0.027064	Biso	1.000000	I
I14	1.0	0.749978	0.539058	0.027064	Biso	1.000000	I
I15	1.0	0.039058	0.750022	0.027064	Biso	1.000000	I
I16	1.0	0.960942	0.249978	0.027064	Biso	1.000000	I
I17	1.0	0.500000	0.000000	0.240346	Biso	1.000000	I
I18	1.0	-0.000000	0.500000	0.759654	Biso	1.000000	I
I19	1.0	-0.000000	0.000000	0.747784	Biso	1.000000	I
I20	1.0	0.500000	0.500000	0.747784	Biso	1.000000	I
I21	1.0	0.500000	0.500000	0.252216	Biso	1.000000	I
I22	1.0	-0.000000	0.000000	0.252216	Biso	1.000000	I
I23	1.0	-0.000000	0.500000	0.262606	Biso	1.000000	I
I24	1.0	0.500000	0.000000	0.737394	Biso	1.000000	I

P1_0.41GPa_tetragonal.cif

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#======================================================================

# CRYSTAL DATA

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_cell_length_c                         12.57000
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_cell_angle_beta                       90
_cell_angle_gamma                      90
_symmetry_space_group_name_H-M         'P 1'
_symmetry_Int_Tables_number            1

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_symmetry_equiv_pos_as_xyz
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loop_
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   _atom_site_occupancy
   _atom_site_fract_x
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   _atom_site_fract_z
   _atom_site_adp_type
   _atom_site_B_iso_or_equiv
   _atom_site_type_symbol
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   H2          1.0     0.671348      0.803620      0.662988     Biso  1.000000 H
   H3          1.0     0.329761      0.190942      0.663715     Biso  1.000000 H
   H4          1.0     0.829492      0.696870      0.702080     Biso  1.000000 H
   H5          1.0     0.217187      0.335672      0.817256     Biso  1.000000 H
   H6          1.0     0.618276      0.775647      0.784061     Biso  1.000000 H
   H7          1.0     0.378726      0.233000      0.782873     Biso  1.000000 H
   H8          1.0     0.774079      0.668284      0.831001     Biso  1.000000 H
   H9          1.0     0.187975      0.195706      0.797038     Biso  1.000000 H
   H10         1.0     0.634195      0.677123      0.694840     Biso  1.000000 H
   H11         1.0     0.358823      0.321286      0.684034     Biso  1.000000 H
   H12         1.0     0.811519      0.803616      0.796945     Biso  1.000000 H
   H13         1.0     0.685961      0.300622      0.811232     Biso  1.000000 H
   H14         1.0     0.184868      0.882618      0.744830     Biso  1.000000 H
   H15         1.0     0.754349      0.121602      0.775468     Biso  1.000000 H
   H16         1.0     0.276253      0.741963      0.850266     Biso  1.000000 H
   H17         1.0     0.755753      0.347809      0.694851     Biso  1.000000 H
   H18         1.0     0.223717      0.822216      0.632606     Biso  1.000000 H
   H19         1.0     0.819951      0.166708      0.665363     Biso  1.000000 H
   H20         1.0     0.309663      0.676867      0.726658     Biso  1.000000 H
   H21         1.0     0.830279      0.298834      0.807415     Biso  1.000000 H
   H22         1.0     0.316777      0.874972      0.715079     Biso  1.000000 H
   H23         1.0     0.685758      0.168772      0.667965     Biso  1.000000 H
   H24         1.0     0.171375      0.689306      0.766699     Biso  1.000000 H
   H25         1.0     0.335635      0.217335      0.317636     Biso  1.000000 H
   H26         1.0     0.775787      0.618257      0.284097     Biso  1.000000 H
   H27         1.0     0.233049      0.378861      0.282899     Biso  1.000000 H
   H28         1.0     0.668169      0.773881      0.331082     Biso  1.000000 H
   H29         1.0     0.290851      0.164609      0.192123     Biso  1.000000 H
   H30         1.0     0.803406      0.671282      0.162916     Biso  1.000000 H
   H31         1.0     0.191088      0.329711      0.163789     Biso  1.000000 H
   H32         1.0     0.696420      0.829246      0.202055     Biso  1.000000 H
   H33         1.0     0.195676      0.188150      0.297369     Biso  1.000000 H
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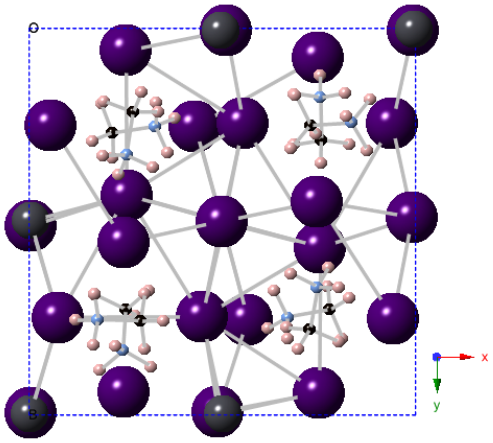

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H36	1.0	0.803366	0.811558	0.296770	Biso	1.000000	H
H37	1.0	0.822690	0.226236	0.131997	Biso	1.000000	H
H38	1.0	0.347925	0.755580	0.195016	Biso	1.000000	H
H39	1.0	0.678497	0.311418	0.229137	Biso	1.000000	H
H40	1.0	0.166875	0.819720	0.165115	Biso	1.000000	H
H41	1.0	0.882832	0.183561	0.243058	Biso	1.000000	H
H42	1.0	0.300584	0.686138	0.311548	Biso	1.000000	H
H43	1.0	0.743169	0.272266	0.351351	Biso	1.000000	H
H44	1.0	0.121628	0.754435	0.275341	Biso	1.000000	H
H45	1.0	0.876309	0.316398	0.216906	Biso	1.000000	H
H46	1.0	0.298837	0.830454	0.307312	Biso	1.000000	H
H47	1.0	0.688950	0.171508	0.263887	Biso	1.000000	H
H48	1.0	0.168928	0.685531	0.168101	Biso	1.000000	H
C1	1.0	0.216309	0.269946	0.759211	Biso	1.000000	C
C2	1.0	0.756659	0.289562	0.760373	Biso	1.000000	C
C3	1.0	0.269954	0.216385	0.259545	Biso	1.000000	C
C4	1.0	0.289604	0.756693	0.260472	Biso	1.000000	C
C5	1.0	0.778949	0.727558	0.766682	Biso	1.000000	C
C6	1.0	0.250895	0.727675	0.768069	Biso	1.000000	C
C7	1.0	0.727319	0.778819	0.266652	Biso	1.000000	C
C8	1.0	0.728483	0.250353	0.268253	Biso	1.000000	C
N1	1.0	0.668810	0.747089	0.724388	Biso	1.000000	N
N2	1.0	0.244044	0.833089	0.712063	Biso	1.000000	N
N3	1.0	0.747001	0.668673	0.224429	Biso	1.000000	N
N4	1.0	0.833780	0.244122	0.211974	Biso	1.000000	N
N5	1.0	0.327927	0.252674	0.719806	Biso	1.000000	N
N6	1.0	0.754031	0.178964	0.715070	Biso	1.000000	N
N7	1.0	0.252762	0.327943	0.219943	Biso	1.000000	N
N8	1.0	0.179068	0.753944	0.215031	Biso	1.000000	N
Pb1	1.0	0.502340	-0.003234	0.494546	Biso	1.000000	Pb
Pb2	1.0	0.004494	0.497692	0.504110	Biso	1.000000	Pb
Pb3	1.0	-0.003677	0.002342	0.004832	Biso	1.000000	Pb
Pb4	1.0	0.499562	0.504387	-0.010446	Biso	1.000000	Pb
Pb5	1.0	0.497547	0.004191	0.003638	Biso	1.000000	Pb
Pb6	1.0	-0.003225	0.502141	-0.005087	Biso	1.000000	Pb
Pb7	1.0	0.002486	-0.003495	0.504898	Biso	1.000000	Pb
Pb8	1.0	0.504830	0.499584	0.489571	Biso	1.000000	Pb
I1	1.0	0.489265	-0.008137	0.752223	Biso	1.000000	I
I2	1.0	0.006291	0.510162	0.750889	Biso	1.000000	I
I3	1.0	-0.006841	0.004709	0.257439	Biso	1.000000	I
I4	1.0	0.500502	0.498862	0.241596	Biso	1.000000	I
I5	1.0	0.509937	0.006351	0.250422	Biso	1.000000	I
I6	1.0	-0.007662	0.489368	0.252694	Biso	1.000000	I
I7	1.0	0.004894	-0.006921	0.757462	Biso	1.000000	I
I8	1.0	0.499037	0.500357	0.741605	Biso	1.000000	I
I9	1.0	0.939740	0.246373	0.508113	Biso	1.000000	I
I10	1.0	0.448227	0.746889	0.514932	Biso	1.000000	I
I11	1.0	0.554606	0.246576	0.522265	Biso	1.000000	I
I12	1.0	0.076564	0.747932	0.484166	Biso	1.000000	I
I13	1.0	0.253908	0.430984	0.487163	Biso	1.000000	I
I14	1.0	0.750872	0.942218	0.531598	Biso	1.000000	I
I15	1.0	0.251829	0.057825	0.518380	Biso	1.000000	I
I16	1.0	0.754193	0.566120	0.494885	Biso	1.000000	I
I17	1.0	0.747769	0.076389	0.984067	Biso	1.000000	I
I18	1.0	0.246644	0.554507	0.022442	Biso	1.000000	I
I19	1.0	0.746936	0.447827	0.015101	Biso	1.000000	I
I20	1.0	0.246179	0.939244	0.007532	Biso	1.000000	I
I21	1.0	0.058028	0.251693	0.018416	Biso	1.000000	I
I22	1.0	0.565995	0.753796	0.994772	Biso	1.000000	I
I23	1.0	0.430647	0.253582	0.987046	Biso	1.000000	I
I24	1.0	0.942145	0.750726	0.031814	Biso	1.000000	I

P4n_0.41GPa_tetragonal.cif

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# CRYSTAL DATA

#----------------------------------------------------------------------

data_VESTA_phase_1


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_cell_length_b                         12.41679
_cell_length_c                         12.57000
_cell_angle_alpha                      90
_cell_angle_beta                       90
_cell_angle_gamma                      90
_symmetry_space_group_name_H-M         'P 1'
_symmetry_Int_Tables_number            1

loop_
_symmetry_equiv_pos_as_xyz
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loop_
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   _atom_site_fract_z
   _atom_site_adp_type
   _atom_site_B_iso_or_equiv
   _atom_site_type_symbol
   H1         1.0     0.184875     0.691231     0.332901     Biso  1.000000 H
   H2         1.0     0.815125     0.308769     0.332901     Biso  1.000000 H
   H3         1.0     0.808769     0.684875     0.332901     Biso  1.000000 H
   H4         1.0     0.191231     0.315125     0.332901     Biso  1.000000 H
   H5         1.0     0.315125     0.808769     0.667099     Biso  1.000000 H
   H6         1.0     0.684875     0.191231     0.667099     Biso  1.000000 H
   H7         1.0     0.691231     0.815125     0.667099     Biso  1.000000 H
   H8         1.0     0.308769     0.184875     0.667099     Biso  1.000000 H
   H9         1.0     0.120753     0.727397     0.218640     Biso  1.000000 H
   H10        1.0     0.879247     0.272603     0.218640     Biso  1.000000 H
   H11        1.0     0.772603     0.620753     0.218640     Biso  1.000000 H
   H12        1.0     0.227397     0.379247     0.218640     Biso  1.000000 H
   H13        1.0     0.379247     0.772603     0.781360     Biso  1.000000 H
   H14        1.0     0.620753     0.227397     0.781360     Biso  1.000000 H
   H15        1.0     0.727397     0.879247     0.781360     Biso  1.000000 H
   H16        1.0     0.272603     0.120753     0.781360     Biso  1.000000 H
   H17        1.0     0.155566     0.820814     0.308519     Biso  1.000000 H
   H18        1.0     0.844434     0.179186     0.308519     Biso  1.000000 H
   H19        1.0     0.679186     0.655566     0.308519     Biso  1.000000 H
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   H21        1.0     0.344434     0.679186     0.691481     Biso  1.000000 H
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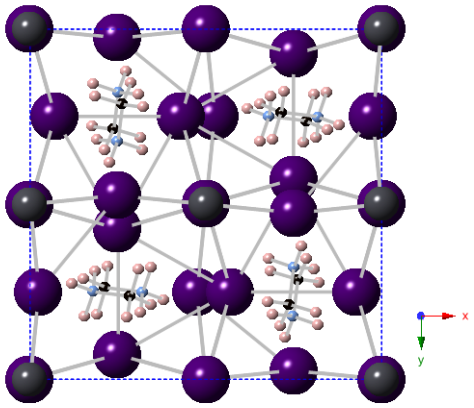

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H42	1.0	0.653962	0.212228	0.276840	Biso	1.000000	H
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H46	1.0	0.846038	0.287772	0.723160	Biso	1.000000	H
H47	1.0	0.787772	0.653962	0.723160	Biso	1.000000	H
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C3	1.0	0.737538	0.785623	0.218550	Biso	1.000000	C
C4	1.0	0.262462	0.214377	0.218550	Biso	1.000000	C
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I7	1.0	0.250014	0.570846	0.495079	Biso	1.000000	I
I8	1.0	0.749986	0.429154	0.495079	Biso	1.000000	I
I9	1.0	0.249996	0.025098	0.966354	Biso	1.000000	I
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I12	1.0	0.525098	0.250004	0.966354	Biso	1.000000	I
I13	1.0	0.250004	0.474902	0.033646	Biso	1.000000	I
I14	1.0	0.749996	0.525098	0.033646	Biso	1.000000	I
I15	1.0	0.025098	0.750004	0.033646	Biso	1.000000	I
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I17	1.0	0.500000	0.000000	0.240442	Biso	1.000000	I
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I19	1.0	-0.000000	0.000000	0.747636	Biso	1.000000	I
I20	1.0	0.500000	0.500000	0.747636	Biso	1.000000	I
I21	1.0	0.500000	0.500000	0.252364	Biso	1.000000	I
I22	1.0	-0.000000	0.000000	0.252364	Biso	1.000000	I
I23	1.0	-0.000000	0.500000	0.262106	Biso	1.000000	I
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P1_0.41GPa_cubic.cif

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# CRYSTAL DATA

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_cell_length_c                         12.41000
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_symmetry_Int_Tables_number            1

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   H16         1.0     0.277231      0.740734      0.851329     Biso  1.000000 H
   H17         1.0     0.755814      0.348043      0.694269     Biso  1.000000 H
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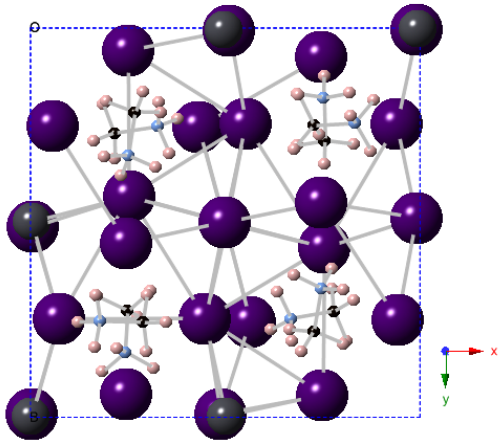

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C7	1.0	0.727588	0.779311	0.266909	Biso	1.000000	C
C8	1.0	0.727868	0.250245	0.268537	Biso	1.000000	C
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I12	1.0	0.074696	0.747715	0.484621	Biso	1.000000	I
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I19	1.0	0.747109	0.448749	0.015052	Biso	1.000000	I
I20	1.0	0.246258	0.940673	0.006895	Biso	1.000000	I
I21	1.0	0.057198	0.251762	0.017333	Biso	1.000000	I
I22	1.0	0.564233	0.754274	0.995365	Biso	1.000000	I
I23	1.0	0.432490	0.254023	0.988328	Biso	1.000000	I
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P4n_0.41GPa_cubic.cif

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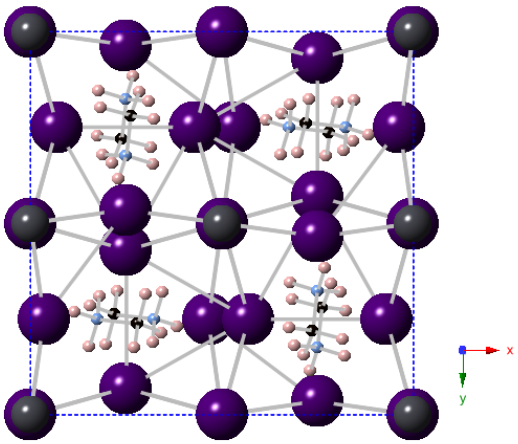

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H38	1.0	0.801145	0.185013	0.818340	Biso	1.000000	H
H39	1.0	0.685013	0.698855	0.818340	Biso	1.000000	H
H40	1.0	0.314987	0.301146	0.818340	Biso	1.000000	H
H41	1.0	0.342990	0.784740	0.278417	Biso	1.000000	H
H42	1.0	0.657010	0.215260	0.278417	Biso	1.000000	H
H43	1.0	0.715260	0.842990	0.278417	Biso	1.000000	H
H44	1.0	0.284740	0.157010	0.278417	Biso	1.000000	H
H45	1.0	0.157010	0.715260	0.721583	Biso	1.000000	H
H46	1.0	0.842990	0.284740	0.721583	Biso	1.000000	H
H47	1.0	0.784740	0.657010	0.721583	Biso	1.000000	H
H48	1.0	0.215260	0.342990	0.721583	Biso	1.000000	H
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C3	1.0	0.737959	0.781021	0.219819	Biso	1.000000	C
C4	1.0	0.262041	0.218979	0.219819	Biso	1.000000	C
C5	1.0	0.218979	0.737959	0.780181	Biso	1.000000	C
C6	1.0	0.781021	0.262041	0.780181	Biso	1.000000	C
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C8	1.0	0.237959	0.281021	0.780181	Biso	1.000000	C
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N3	1.0	0.749675	0.675944	0.276698	Biso	1.000000	N
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N5	1.0	0.324056	0.749675	0.723302	Biso	1.000000	N
N6	1.0	0.675944	0.250325	0.723302	Biso	1.000000	N
N7	1.0	0.750325	0.824056	0.723302	Biso	1.000000	N
N8	1.0	0.249675	0.175944	0.723302	Biso	1.000000	N
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Pb3	1.0	0.500000	0.000000	-0.005096	Biso	1.000000	Pb
Pb4	1.0	0.000000	0.500000	0.005096	Biso	1.000000	Pb
Pb5	1.0	0.500000	0.000000	0.487102	Biso	1.000000	Pb
Pb6	1.0	0.000000	0.500000	0.512898	Biso	1.000000	Pb
Pb7	1.0	0.000000	0.000000	0.000000	Biso	1.000000	Pb
Pb8	1.0	0.500000	0.500000	0.000000	Biso	1.000000	Pb
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I2	1.0	0.569911	0.750229	0.502394	Biso	1.000000	I
I3	1.0	0.250229	0.930089	0.502394	Biso	1.000000	I
I4	1.0	0.749771	0.069911	0.502394	Biso	1.000000	I
I5	1.0	0.069911	0.250229	0.497606	Biso	1.000000	I
I6	1.0	0.930089	0.749771	0.497606	Biso	1.000000	I
I7	1.0	0.249771	0.569911	0.497606	Biso	1.000000	I
I8	1.0	0.750229	0.430089	0.497606	Biso	1.000000	I
I9	1.0	0.249923	0.035319	0.974264	Biso	1.000000	I
I10	1.0	0.750077	0.964681	0.974264	Biso	1.000000	I
I11	1.0	0.464681	0.749923	0.974264	Biso	1.000000	I
I12	1.0	0.535319	0.250077	0.974264	Biso	1.000000	I
I13	1.0	0.250077	0.464681	0.025736	Biso	1.000000	I
I14	1.0	0.749923	0.535319	0.025736	Biso	1.000000	I
I15	1.0	0.035319	0.750077	0.025736	Biso	1.000000	I
I16	1.0	0.964681	0.249923	0.025736	Biso	1.000000	I
I17	1.0	0.500000	0.000000	0.241480	Biso	1.000000	I
I18	1.0	0.000000	0.500000	0.758520	Biso	1.000000	I
I19	1.0	0.000000	0.000000	0.748102	Biso	1.000000	I
I20	1.0	0.500000	0.500000	0.748102	Biso	1.000000	I
I21	1.0	0.500000	0.500000	0.251898	Biso	1.000000	I
I22	1.0	0.000000	0.000000	0.251898	Biso	1.000000	I
I23	1.0	0.000000	0.500000	0.261436	Biso	1.000000	I
I24	1.0	0.500000	0.000000	0.738564	Biso	1.000000	I

P1_1.04GPa_cubic.cif

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# CRYSTAL DATA

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_symmetry_Int_Tables_number            1

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   _atom_site_fract_x
   _atom_site_fract_y
   _atom_site_fract_z
   _atom_site_adp_type
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   H4         1.0     0.821267      0.695528      0.715865     Biso  1.000000 H
   H5         1.0     0.189651      0.333277      0.778858     Biso  1.000000 H
   H6         1.0     0.603319      0.770216      0.795352     Biso  1.000000 H
   H7         1.0     0.372711      0.255426      0.762391     Biso  1.000000 H
   H8         1.0     0.766015      0.671033      0.850227     Biso  1.000000 H
   H9         1.0     0.193774      0.190756      0.813331     Biso  1.000000 H
   H10        1.0     0.622766      0.662979      0.712645     Biso  1.000000 H
   H11        1.0     0.325673      0.300238      0.639482     Biso  1.000000 H
   H12        1.0     0.796210      0.807978      0.806852     Biso  1.000000 H
   H13        1.0     0.708523      0.326458      0.794318     Biso  1.000000 H
   H14        1.0     0.183337      0.867830      0.746393     Biso  1.000000 H
   H15        1.0     0.754515      0.135019      0.783310     Biso  1.000000 H
   H16        1.0     0.305476      0.768262      0.869512     Biso  1.000000 H
   H17        1.0     0.785474      0.350178      0.671484     Biso  1.000000 H
   H18        1.0     0.238516      0.805529      0.637643     Biso  1.000000 H
   H19        1.0     0.830156      0.156732      0.668387     Biso  1.000000 H
   H20        1.0     0.364545      0.702474      0.751510     Biso  1.000000 H
   H21        1.0     0.853715      0.307348      0.794969     Biso  1.000000 H
   H22        1.0     0.315140      0.890465      0.714190     Biso  1.000000 H
   H23        1.0     0.694723      0.176222      0.664439     Biso  1.000000 H
   H24        1.0     0.225043      0.676019      0.788558     Biso  1.000000 H
   H25        1.0     0.333640      0.190071      0.279218     Biso  1.000000 H
   H26        1.0     0.770513      0.603766      0.295977     Biso  1.000000 H
   H27        1.0     0.255493      0.372906      0.262019     Biso  1.000000 H
   H28        1.0     0.670896      0.766445      0.349983     Biso  1.000000 H
   H29        1.0     0.233332      0.143367      0.182126     Biso  1.000000 H
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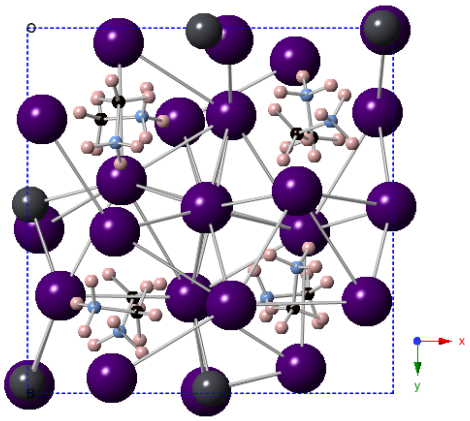

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H37	1.0	0.806076	0.238333	0.137661	Biso	1.000000	H
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H39	1.0	0.701538	0.363061	0.251404	Biso	1.000000	H
H40	1.0	0.157120	0.830105	0.167861	Biso	1.000000	H
H41	1.0	0.869141	0.183914	0.246378	Biso	1.000000	H
H42	1.0	0.326723	0.708940	0.294409	Biso	1.000000	H
H43	1.0	0.768563	0.305485	0.369458	Biso	1.000000	H
H44	1.0	0.135386	0.754773	0.282999	Biso	1.000000	H
H45	1.0	0.890369	0.315879	0.214018	Biso	1.000000	H
H46	1.0	0.307815	0.854156	0.294092	Biso	1.000000	H
H47	1.0	0.677219	0.223375	0.289177	Biso	1.000000	H
H48	1.0	0.176606	0.694660	0.164290	Biso	1.000000	H
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C2	1.0	0.779077	0.300345	0.745799	Biso	1.000000	C
C3	1.0	0.250706	0.202494	0.247400	Biso	1.000000	C
C4	1.0	0.300727	0.779210	0.245417	Biso	1.000000	C
C5	1.0	0.767836	0.727199	0.780406	Biso	1.000000	C
C6	1.0	0.290064	0.737600	0.786838	Biso	1.000000	C
C7	1.0	0.726939	0.768081	0.280062	Biso	1.000000	C
C8	1.0	0.737860	0.289268	0.286953	Biso	1.000000	C
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N2	1.0	0.254382	0.830486	0.717285	Biso	1.000000	N
N3	1.0	0.738240	0.655283	0.236363	Biso	1.000000	N
N4	1.0	0.831013	0.254517	0.217248	Biso	1.000000	N
N5	1.0	0.314622	0.242743	0.701560	Biso	1.000000	N
N6	1.0	0.763916	0.184200	0.713988	Biso	1.000000	N
N7	1.0	0.242858	0.314557	0.201447	Biso	1.000000	N
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Pb2	1.0	0.008674	0.483144	0.506921	Biso	1.000000	Pb
Pb3	1.0	-0.027837	0.000352	0.001519	Biso	1.000000	Pb
Pb4	1.0	0.490879	0.509493	-0.007303	Biso	1.000000	Pb
Pb5	1.0	0.483209	0.008294	0.006967	Biso	1.000000	Pb
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I2	1.0	0.033202	0.551489	0.748704	Biso	1.000000	I
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I4	1.0	0.489072	0.494543	0.243803	Biso	1.000000	I
I5	1.0	0.550910	0.032904	0.248851	Biso	1.000000	I
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I10	1.0	0.447287	0.738135	0.511464	Biso	1.000000	I
I11	1.0	0.557179	0.238591	0.525470	Biso	1.000000	I
I12	1.0	0.091987	0.732052	0.481231	Biso	1.000000	I
I13	1.0	0.258661	0.417694	0.477475	Biso	1.000000	I
I14	1.0	0.749391	0.930752	0.542977	Biso	1.000000	I
I15	1.0	0.250852	0.040418	0.501306	Biso	1.000000	I
I16	1.0	0.759494	0.559224	0.510499	Biso	1.000000	I
I17	1.0	0.732148	0.091742	0.981687	Biso	1.000000	I
I18	1.0	0.238858	0.557117	0.025449	Biso	1.000000	I
I19	1.0	0.738483	0.447336	0.011635	Biso	1.000000	I
I20	1.0	0.230874	0.957630	0.006931	Biso	1.000000	I
I21	1.0	0.040534	0.251057	0.000985	Biso	1.000000	I
I22	1.0	0.559397	0.759175	0.010110	Biso	1.000000	I
I23	1.0	0.417933	0.258397	0.977601	Biso	1.000000	I
I24	1.0	0.930763	0.749529	0.043191	Biso	1.000000	I

P4n_1.04GPa_cubic.cif

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# CRYSTAL DATA

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   H5          1.0     0.336371      0.838476      0.734195     Biso  1.000000 H
   H6          1.0     0.663629      0.161524      0.734195     Biso  1.000000 H
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   H27         1.0     0.613753      0.754737      0.235929     Biso  1.000000 H
   H28         1.0     0.386247      0.245263      0.235929     Biso  1.000000 H
   H29         1.0     0.245263      0.613753      0.764071     Biso  1.000000 H
   H30         1.0     0.754737      0.386247      0.764071     Biso  1.000000 H
   H31         1.0     0.886247      0.745263      0.764071     Biso  1.000000 H
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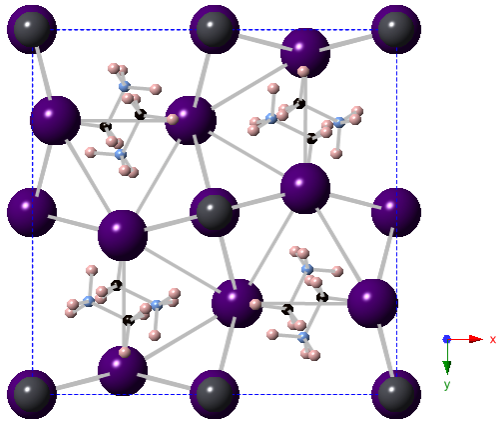

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H39	1.0	0.763575	0.687832	0.821103	Biso	1.000000	H
H40	1.0	0.236425	0.312168	0.821103	Biso	1.000000	H
H41	1.0	0.307928	0.782139	0.324907	Biso	1.000000	H
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H44	1.0	0.282139	0.192072	0.324907	Biso	1.000000	H
H45	1.0	0.192072	0.717861	0.675093	Biso	1.000000	H
H46	1.0	0.807928	0.282139	0.675093	Biso	1.000000	H
H47	1.0	0.782139	0.692072	0.675093	Biso	1.000000	H
H48	1.0	0.217861	0.307928	0.675093	Biso	1.000000	H
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C2	1.0	0.733880	0.201722	0.247424	Biso	1.000000	C
C3	1.0	0.701722	0.766120	0.247424	Biso	1.000000	C
C4	1.0	0.298278	0.233880	0.247424	Biso	1.000000	C
C5	1.0	0.233880	0.701722	0.752576	Biso	1.000000	C
C6	1.0	0.766120	0.298278	0.752576	Biso	1.000000	C
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C8	1.0	0.201722	0.266120	0.752576	Biso	1.000000	C
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N2	1.0	0.843153	0.255149	0.251089	Biso	1.000000	N
N3	1.0	0.755149	0.656847	0.251089	Biso	1.000000	N
N4	1.0	0.244851	0.343153	0.251089	Biso	1.000000	N
N5	1.0	0.343153	0.755149	0.748911	Biso	1.000000	N
N6	1.0	0.656847	0.244851	0.748911	Biso	1.000000	N
N7	1.0	0.744851	0.843153	0.748911	Biso	1.000000	N
N8	1.0	0.255149	0.156847	0.748911	Biso	1.000000	N
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Pb3	1.0	0.500000	-0.000000	0.004075	Biso	1.000000	Pb
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Pb5	1.0	0.500000	-0.000000	0.496244	Biso	1.000000	Pb
Pb6	1.0	-0.000000	0.500000	0.503756	Biso	1.000000	Pb
Pb7	1.0	-0.000000	-0.000000	-0.000000	Biso	1.000000	Pb
Pb8	1.0	0.500000	0.500000	-0.000000	Biso	1.000000	Pb
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I2	1.0	0.565902	0.749810	0.528938	Biso	1.000000	I
I3	1.0	0.249810	0.934098	0.528938	Biso	1.000000	I
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I6	1.0	0.934098	0.750190	0.471062	Biso	1.000000	I
I7	1.0	0.250190	0.565902	0.471062	Biso	1.000000	I
I8	1.0	0.749810	0.434098	0.471062	Biso	1.000000	I
I9	1.0	0.250178	0.938067	0.969810	Biso	1.000000	I
I10	1.0	0.749822	0.061933	0.969810	Biso	1.000000	I
I11	1.0	0.561933	0.750178	0.969810	Biso	1.000000	I
I12	1.0	0.438067	0.249822	0.969810	Biso	1.000000	I
I13	1.0	0.249822	0.561933	0.030190	Biso	1.000000	I
I14	1.0	0.750178	0.438067	0.030190	Biso	1.000000	I
I15	1.0	0.938067	0.749822	0.030190	Biso	1.000000	I
I16	1.0	0.061933	0.250178	0.030190	Biso	1.000000	I
I17	1.0	0.500000	-0.000000	0.250346	Biso	1.000000	I
I18	1.0	-0.000000	0.500000	0.749654	Biso	1.000000	I
I19	1.0	-0.000000	-0.000000	0.749688	Biso	1.000000	I
I20	1.0	0.500000	0.500000	0.749688	Biso	1.000000	I
I21	1.0	0.500000	0.500000	0.250312	Biso	1.000000	I
I22	1.0	-0.000000	-0.000000	0.250312	Biso	1.000000	I
I23	1.0	-0.000000	0.500000	0.250442	Biso	1.000000	I
I24	1.0	0.500000	-0.000000	0.749558	Biso	1.000000	I

P1_1.95GPa_cubic.cif

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# CRYSTAL DATA

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   H3         1.0     0.332555      0.162503      0.676479     Biso  1.000000 H
   H4         1.0     0.822790      0.694307      0.717864     Biso  1.000000 H
   H5         1.0     0.189152      0.334002      0.778793     Biso  1.000000 H
   H6         1.0     0.603066      0.774757      0.791418     Biso  1.000000 H
   H7         1.0     0.373362      0.257194      0.769197     Biso  1.000000 H
   H8         1.0     0.766246      0.676078      0.853476     Biso  1.000000 H
   H9         1.0     0.191961      0.191399      0.816950     Biso  1.000000 H
   H10        1.0     0.622638      0.660798      0.716316     Biso  1.000000 H
   H11        1.0     0.329255      0.295579      0.641958     Biso  1.000000 H
   H12        1.0     0.796805      0.811735      0.803630     Biso  1.000000 H
   H13        1.0     0.722644      0.328645      0.798222     Biso  1.000000 H
   H14        1.0     0.185119      0.861869      0.755746     Biso  1.000000 H
   H15        1.0     0.754136      0.134444      0.777937     Biso  1.000000 H
   H16        1.0     0.321687      0.764611      0.867164     Biso  1.000000 H
   H17        1.0     0.796014      0.352191      0.672262     Biso  1.000000 H
   H18        1.0     0.227331      0.796247      0.641967     Biso  1.000000 H
   H19        1.0     0.828400      0.154738      0.660784     Biso  1.000000 H
   H20        1.0     0.366033      0.694534      0.743943     Biso  1.000000 H
   H21        1.0     0.867332      0.299912      0.791284     Biso  1.000000 H
   H22        1.0     0.312753      0.883543      0.708353     Biso  1.000000 H
   H23        1.0     0.693774      0.183761      0.661570     Biso  1.000000 H
   H24        1.0     0.231024      0.670246      0.798492     Biso  1.000000 H
   H25        1.0     0.334576      0.189651      0.278982     Biso  1.000000 H
   H26        1.0     0.774081      0.603075      0.291648     Biso  1.000000 H
   H27        1.0     0.256570      0.373377      0.269089     Biso  1.000000 H
   H28        1.0     0.675994      0.766494      0.353476     Biso  1.000000 H
   H29        1.0     0.231476      0.145013      0.182375     Biso  1.000000 H
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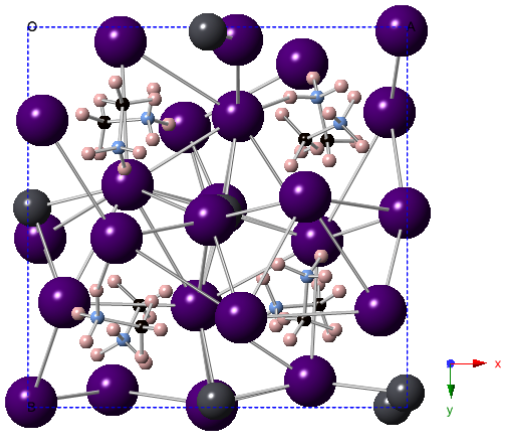

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H41	1.0	0.863191	0.185268	0.255335	Biso	1.000000 H
H42	1.0	0.328965	0.721855	0.297470	Biso	1.000000 H
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H45	1.0	0.883929	0.313238	0.208425	Biso	1.000000 H
H46	1.0	0.300940	0.866693	0.290879	Biso	1.000000 H
H47	1.0	0.671419	0.229493	0.298647	Biso	1.000000 H
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C3	1.0	0.250316	0.202556	0.249397	Biso	1.000000 C
C4	1.0	0.300102	0.789043	0.244810	Biso	1.000000 C
C5	1.0	0.768456	0.729253	0.780683	Biso	1.000000 C
C6	1.0	0.296112	0.731554	0.787271	Biso	1.000000 C
C7	1.0	0.729085	0.768547	0.280617	Biso	1.000000 C
C8	1.0	0.732094	0.295175	0.287400	Biso	1.000000 C
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N2	1.0	0.252546	0.823246	0.719334	Biso	1.000000 N
N3	1.0	0.737468	0.655607	0.234776	Biso	1.000000 N
N4	1.0	0.824075	0.252515	0.219249	Biso	1.000000 N
N5	1.0	0.316853	0.240797	0.706922	Biso	1.000000 N
N6	1.0	0.765259	0.185413	0.709751	Biso	1.000000 N
N7	1.0	0.240570	0.316664	0.206927	Biso	1.000000 N
N8	1.0	0.185613	0.765344	0.209614	Biso	1.000000 N
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Pb3	1.0	0.962819	0.997638	0.996179	Biso	1.000000 Pb
Pb4	1.0	0.487796	0.517239	0.989387	Biso	1.000000 Pb
Pb5	1.0	0.476286	0.012198	0.008593	Biso	1.000000 Pb
Pb6	1.0	0.984400	0.497981	0.989047	Biso	1.000000 Pb
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I2	1.0	0.033945	0.553992	0.749675	Biso	1.000000 I
I3	1.0	0.987478	0.009404	0.248379	Biso	1.000000 I
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I8	1.0	0.510153	0.479625	0.741864	Biso	1.000000 I
I9	1.0	0.954656	0.225092	0.498342	Biso	1.000000 I
I10	1.0	0.447166	0.733737	0.512769	Biso	1.000000 I
I11	1.0	0.554928	0.234906	0.524839	Biso	1.000000 I
I12	1.0	0.097898	0.725731	0.479037	Biso	1.000000 I
I13	1.0	0.263299	0.414936	0.483178	Biso	1.000000 I
I14	1.0	0.745907	0.931234	0.541433	Biso	1.000000 I
I15	1.0	0.246427	0.040167	0.503848	Biso	1.000000 I
I16	1.0	0.765070	0.562965	0.510352	Biso	1.000000 I
I17	1.0	0.725492	0.098166	0.979178	Biso	1.000000 I
I18	1.0	0.234644	0.554928	0.024795	Biso	1.000000 I
I19	1.0	0.733482	0.447153	0.013292	Biso	1.000000 I
I20	1.0	0.224950	0.954416	0.997862	Biso	1.000000 I
I21	1.0	0.040240	0.246769	0.003313	Biso	1.000000 I
I22	1.0	0.562781	0.765188	0.010592	Biso	1.000000 I
I23	1.0	0.414671	0.263461	0.982857	Biso	1.000000 I
I24	1.0	0.931025	0.746319	0.041997	Biso	1.000000 I

P4n_1.95GPa_cubic.cif

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   H4         1.0     0.160946     0.335013     0.265693     Biso  1.000000 H
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   H6         1.0     0.664987     0.160946     0.734307     Biso  1.000000 H
   H7         1.0     0.660946     0.835013     0.734307     Biso  1.000000 H
   H8         1.0     0.339054     0.164987     0.734307     Biso  1.000000 H
   H9         1.0     0.115133     0.753278     0.176520     Biso  1.000000 H
   H10        1.0     0.884867     0.246722     0.176520     Biso  1.000000 H
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   H27        1.0     0.612252     0.755434     0.236946     Biso  1.000000 H
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   H31        1.0     0.887748     0.744566     0.763054     Biso  1.000000 H
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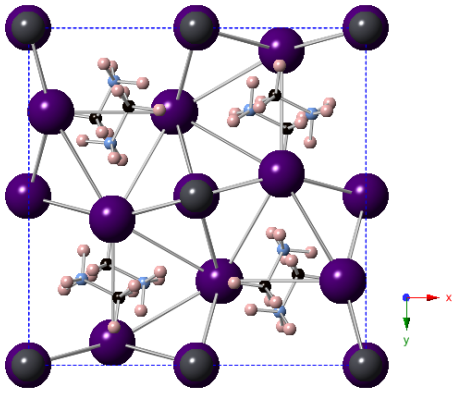

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H39	1.0	0.765191	0.685534	0.821474	Biso	1.000000	H
H40	1.0	0.234809	0.314466	0.821474	Biso	1.000000	H
H41	1.0	0.309357	0.782356	0.325796	Biso	1.000000	H
H42	1.0	0.690643	0.217644	0.325796	Biso	1.000000	H
H43	1.0	0.717644	0.809357	0.325796	Biso	1.000000	H
H44	1.0	0.282356	0.190643	0.325796	Biso	1.000000	H
H45	1.0	0.190643	0.717644	0.674204	Biso	1.000000	H
H46	1.0	0.809357	0.282356	0.674204	Biso	1.000000	H
H47	1.0	0.782356	0.690643	0.674204	Biso	1.000000	H
H48	1.0	0.217644	0.309357	0.674204	Biso	1.000000	H
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C3	1.0	0.700841	0.767590	0.247698	Biso	1.000000	C
C4	1.0	0.299159	0.232410	0.247698	Biso	1.000000	C
C5	1.0	0.232410	0.700841	0.752302	Biso	1.000000	C
C6	1.0	0.767590	0.299159	0.752302	Biso	1.000000	C
C7	1.0	0.799159	0.732410	0.752302	Biso	1.000000	C
C8	1.0	0.200841	0.267590	0.752302	Biso	1.000000	C
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N2	1.0	0.842081	0.255246	0.250320	Biso	1.000000	N
N3	1.0	0.755246	0.657919	0.250320	Biso	1.000000	N
N4	1.0	0.244754	0.342081	0.250320	Biso	1.000000	N
N5	1.0	0.342081	0.755246	0.749680	Biso	1.000000	N
N6	1.0	0.657919	0.244754	0.749680	Biso	1.000000	N
N7	1.0	0.744754	0.842081	0.749680	Biso	1.000000	N
N8	1.0	0.255246	0.157919	0.749680	Biso	1.000000	N
Pb1	1.0	-0.000000	0.000000	0.500000	Biso	1.000000	Pb
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Pb3	1.0	0.500000	0.000000	0.004569	Biso	1.000000	Pb
Pb4	1.0	-0.000000	0.500000	0.995431	Biso	1.000000	Pb
Pb5	1.0	0.500000	0.000000	0.497163	Biso	1.000000	Pb
Pb6	1.0	-0.000000	0.500000	0.502837	Biso	1.000000	Pb
Pb7	1.0	-0.000000	0.000000	-0.000000	Biso	1.000000	Pb
Pb8	1.0	0.500000	0.500000	-0.000000	Biso	1.000000	Pb
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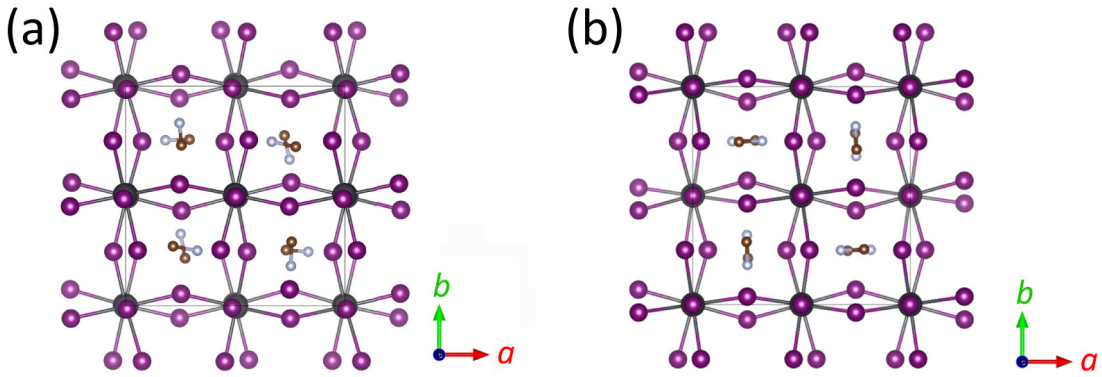
I2	1.0	0.568787	0.749627	0.529800	Biso	1.000000	I
I3	1.0	0.249627	0.931213	0.529800	Biso	1.000000	I
I4	1.0	0.750373	0.068787	0.529800	Biso	1.000000	I
I5	1.0	0.068787	0.249627	0.470200	Biso	1.000000	I
I6	1.0	0.931213	0.750373	0.470200	Biso	1.000000	I
I7	1.0	0.250373	0.568787	0.470200	Biso	1.000000	I
I8	1.0	0.749627	0.431213	0.470200	Biso	1.000000	I
I9	1.0	0.250080	0.935159	0.969672	Biso	1.000000	I
I10	1.0	0.749920	0.064841	0.969672	Biso	1.000000	I
I11	1.0	0.564841	0.750080	0.969672	Biso	1.000000	I
I12	1.0	0.435159	0.249920	0.969672	Biso	1.000000	I
I13	1.0	0.249920	0.564841	0.030328	Biso	1.000000	I
I14	1.0	0.750080	0.435159	0.030328	Biso	1.000000	I
I15	1.0	0.935159	0.749920	0.030328	Biso	1.000000	I
I16	1.0	0.064841	0.250080	0.030328	Biso	1.000000	I
I17	1.0	0.500000	0.000000	0.250805	Biso	1.000000	I
I18	1.0	-0.000000	0.500000	0.749195	Biso	1.000000	I
I19	1.0	-0.000000	0.000000	0.749839	Biso	1.000000	I
I20	1.0	0.500000	0.500000	0.749839	Biso	1.000000	I
I21	1.0	0.500000	0.500000	0.250161	Biso	1.000000	I
I22	1.0	-0.000000	0.000000	0.250161	Biso	1.000000	I
I23	1.0	-0.000000	0.500000	0.249696	Biso	1.000000	I
I24	1.0	0.500000	0.000000	0.750304	Biso	1.000000	I

Table S3. Peak wavelength of $MAPbI_3$ photoluminescence spectra (Figure 4) collected under compression and their corresponding estimated bandgaps.

Pressure(GPa)	Wavelength(nm)	Bandgap(eV)
1.95	732.1	1.693
1.37	737.3	1.682
1.04	748.2	1.657
0.80	749.5	1.654
0.41	754.7	1.643
0.30	772.1	1.606
0.16	768.7	1.613
0.11	765.1	1.621
0.05	764.8	1.621
~0	764.1	1.623

Fig. S8. Models for tetragonal and cubic phases of $MAPbI_3$. With explicit MA cations, symmetry is significantly lowered by orientations of C-N dipole and rotation of XH_3 groups. To model high symmetry I4/mcm and $Im\bar{3}$, we fixed the lattice parameters to experimental values, while all atomic positions were relaxed with P1 space group of no symmetry (a), or with a space group of P4/n (b) derived from the orthorhombic phase. The two models are energetically close, with (a) P1 of lower energy. The resulting bandgaps were averaged over the two models according to Boltzmann distribution at room temperature.



H atoms are not shown for simpler view.

Table S4. The predicted bandgaps E_g of $MAPbI_3$ with the two models P1 and P4/n for tetragonal and cubic phases, and the energy difference ΔE with the resulting ratios of structures, according to the Boltzmann distribution at room temperature.

P (GPa)	E_g (eV)				ΔE (eV/$MAPbI_3$)				Ratio				Averaged E_g (eV)
	Tetragonal		Cubic		Tetragonal		Cubic		Tetragonal		Cubic		
	P1	P4/n	P1	P4/n	P1	P4/n	P1	P4/n	P1	P4/n	P1	P4/n	
0	1.695	1.607			0.00000	0.02844			1	0.3306			1.67
0.30	1.659	1.497			0.00000	0.02594			1	0.3643			1.62
0.41	1.649	1.519	1.571	1.413	0.00000	0.02687	0.01914	0.03663	1	0.3514	0.4748	0.2403	1.58
1.04			1.703	1.542			0.00000	0.03177			1	0.2904	1.67
1.95			1.814	1.516			0.00000	0.03052			1	0.3049	1.74

II. Characterization and Fitting Software:

Synchrotron XRD and PL Characterization:

High Pressure Processing: The samples were loaded into a diamond anvil cell (DAC) for separate *in-situ* high pressure XRD runs. Stainless gaskets were pre-indented to reduce the thickness from 250 μm down to ~100 μm. A 200 μm diameter hole was drilled and served as the sample chamber. The samples were loaded into the gasket hole and then several small ruby chips were randomly distributed on the top of the samples for monitoring pressure. A laser-excited ruby fluorescence technique was used to measure the variation of the pressure, at which X-ray diffraction and photoluminescence were performed simultaneously. The optical images were taken from microscope directly at various pressures.

X-ray Diffraction Measurement: The X-ray diffraction was collected at B1 station, Cornell High Energy Synchrotron Source (CHESS), Cornell University. A monochromatic x-ray with the energy of 25.514 keV was collimated using a double pinhole-aligned circular tube into small x-ray beam with a diameter of 100 microns. X-ray scattering signals from the samples were collected using a large area Mar345 detector. The sample-to-detector distance and other detector sitting parameters were calibrated using the powder standard of CeO_2. The raw two-dimensional (2D) images were integrated and analyzed by the Fit2D[S2] package. Photoluminescence Characterization: The laser-excited photoluminescence spectra were recorded at Princeton Acton SP-300i system. The samples loaded in DAC were measured under compression or decompression as soon as each diffraction pattern was recorded. A 532 nm diode laser was used for excitation and the emitted light was collected through the spectrometer with 1200g/mm grating in the exposure time of 3s. In each snapshot, the collected PL spectrum covers only a very narrow wavelength range (40 nm), so the full spectrum presented in this work was technically synthesized by a feasible connection of several snapshots collected at nearby but different wavelength

range. This data processing technically involved slight adjustment of background intensities, but no modification was made on the peak position and intensity in each spectrum.

Fitting Software:

Pawley fitting of the lattice parameters and refinement of the atomic positions were carried out using a Topas (version 3) software package (1999-2000 Bruker AXS).

III. References:

(S1) Toby, B. H. *Powder Diffr.* **2007**, *21*, 67-70.

(S2) Hammersley, A. P. *ESRF97HA02T, "FIT2D: An Introduction and Overview"*, 1997.